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VALIDATION AND SENSITIVITY ANALYSIS OF THE GAUSSIAN PLUME MULTIPLE-SOURCE URBAN DIFFUSION MODEL

FINAL REPORT

for

Division of Meteorology

Environmental Protection Agency
National Environmental Research Center
Research Triangle Park, N.C. 27711

under

Contract Number CPA 70-94

by

Robert C. Koch
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The analysis and results are presented of a program of validation and sensitivity analysis of the steady-state Gaussian plume type of urban diffusion model. A definition is developed of the fundamental short-term steady-state model and its various modes of implementation, in terms of emission and environmental input parameters, and of calculational modes. A set of computer programs developed especially for validation and sensitivity study purposes is described. Comparisons were made of short-term and long-term concentration predictions from the model, with comparable measured SO_2 concentrations covering three months of two-hour values at ten locations in St. Louis, and one month of one-hour values at eight locations in Chicago. Hourly estimates of meteorological and emission parameters were used. Individual short-term model results (one- to two-hour periods) show large deviations from the observed concentrations, but the frequency distributions of calculated ~~short~~-term concentrations over a month or a season compare quite well with the comparable frequency distributions of observed concentrations. No single factor could be found which accounts for a significant fraction of the individual deviations. Predicted long-term concentrations show consistently good agreement with observations, as contrasted with the significant overestimation usually found in other model implementations. A technique is proposed for calculating the long-term estimates which obviates the need to calculate every short-term concentration in the period. A sampling process is used in which a statistically selected set of as few as five to ten percent of the short-term periods is employed, and the representativeness of the distribution is maintained. The insensitivity of the model concentrations to the parameters of wind speed profile parameter value, and the distribution of area source emission heights, is demonstrated. Quantitative description is given of the sensitivity of the model to the following parameters: changes in spatial variability in emissions, vertical diffusion parameter, pollutant half-life, wind speed, mixing ceiling, wind direction, and downwind variation in emission rates.

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PREFACE

This final report under Contract Number CPA-70-94, entitled "Sensitivity Analysis and Evaluation of Multiple-Source Urban Air Pollution Diffusion Models," represents work originally undertaken for the National Air Pollution Control Administration, continued under The Air Pollution Control Office, and completed under the direction of the Environmental Protection Agency (EPA). The guidance and technical direction of the government project officer, Mr. K. L. Calder, of the Division of Meteorology, National Environmental Research Center, Research Triangle Park, EPA, was particularly helpful in the execution of this study. Personnel at GEOMET who contributed significantly to the work reported here include Mr. Douglas J. Pelton, Mr. Martin W. Chandler and Mr. Isadore Enger.

SUMMARY

This report, submitted by GEOMET to the National Environmental Research Center, presents the analysis and results of a program of validation and sensitivity analysis of the steady-state Gaussian plume type of urban diffusion model.

The report develops a careful definition of the fundamental short-term steady-state model and its various modes of implementation, in terms of emission and environmental input parameters, and of calculational modes. A set of computer programs developed especially for validation and sensitivity study purposes is described.

The validation study consists of a variety of comparisons of short-term and long-term concentration predictions from the model, with comparable measured SO_2 concentrations covering three months of two-hour values at ten locations in St. Louis, and one month of one-hour values at eight locations in Chicago. The predictions use hourly estimates of meteorological and emission parameters. The atmospheric stability is estimated from hourly weather observations from an adjacent airport using the McElroy-Pooler diffusion parameters based on Turner's definitions of stability categories. The mixing layer ceiling is estimated from radiosonde observations taken twice daily from remote locations (100 to 200 miles away). The wind speed and direction are hourly averages of several continuous records. The emission rates of the largest sources are identified and located individually. For other sources a mean emission rate per unit area is estimated for a square gridwork of points with a one-mile spacing between adjacent points. Each emission rate is related to hourly estimates of space heating

and other operating requirements. No "calibration" or other adjustment of the inputs or output concentrations is employed anywhere in the analysis.

Individual short-term model results (one- to two-hour periods) show large deviations from the observed concentrations, but the frequency distributions of calculated short-term concentrations over a month or a season compare quite well with the comparable frequency distributions of observed concentrations. No single factor could be found which accounts for a significant fraction of the individual deviations. Predicted long-term concentrations show consistently good agreement with observations, as contrasted with the significant overestimation usually found in other model implementations.

A technique is proposed for calculating the long-term estimates which obviates the need to calculate every short-term concentration in the period. A sampling process is used in which a statistically selected set of as few as five to ten percent of the short-term periods is employed, and the representativeness of the distribution is maintained.

In the sensitivity analysis, the insensitivity of the model concentrations to the parameters of wind speed profile parameter value, and the distribution of area source emission heights, is demonstrated. Quantitative description is given of the sensitivity of the model to the following parameters: changes in spatial variability in emissions, vertical diffusion parameter, pollutant half-life, wind speed, mixing ceiling, wind direction, and downwind variation in emission rates.

Finally, recommendations are made on implementation and use of the model described herein, and for further study in special problem areas highlighted by the study.

Section 1.0

INTRODUCTION

In recent years considerable emphasis has been placed on the development of meteorological models for analysis and prediction of the transport and diffusion of pollutants in urban and surrounding suburban regions. The resulting models range in complexity from simple, ventilated-box models to Gaussian puff trajectory models and complex models based on the eddy diffusivity concept. The most commonly used meteorological model is based on the steady-state Gaussian plume concept and lies, in complexity, somewhere between the simple box model and the Gaussian puff trajectory model. Although variations exist in the way this model has been implemented (for examples, see Appendix A), there is only one basic Gaussian plume model. The generality of this model and its application to urban diffusion analysis has been described by Calder (1970). This basic model has been shown to be valid over downwind travel distances of up to a few hundred kilometers (e.g., see Slade (ed.), 1968 and Pasquill, 1962). Since 1 to 50 kilometers is the distance scale of primary interest in studying urban air pollution problems and since a great deal of experimental work has been devoted to defining parameters for the Gaussian plume model, this concept has been the principal one used to analyze urban air pollution problems.

For a review of urban model developments the reader is referred to papers from a recent symposium on modeling (Stern (ed.), 1970) and recent conference papers (e.g., American Meteorological Society, Raleigh, North Carolina, April 5-9, 1971, and International Union of Air Pollution

Prevention Associations, Washington, D.C., December 6-11, 1970). The Environmental Protection Agency, in its responsibility for directing the development of new urban diffusion models, needs information on how accurately the currently most-used type of model, the "Gaussian plume," can provide estimates of air quality. The validation and sensitivity analysis in this report provides a quantitative description of the capabilities and limitations inherent in the steady-state Gaussian plume type of urban diffusion model.

This report discusses the model structure, the inputs necessary for its implementation, the computer implementation of the model for this study, the results of extensive validation comparisons with two major sets of urban air pollution data in both short-term and long-term applications, the results of extensive sensitivity analyses, and conclusions and recommendations. Appendices contain detailed descriptions of the input data, computer programs, and validation and sensitivity results in the form of computer printouts.

Section 2.0

THE GAUSSIAN PLUME TYPE OF URBAN DIFFUSION MODEL

The Gaussian plume model describes the field of concentrations of airborne pollutants which undergo negligible gravitational settling and which originate from a point source. The concentration field is defined over a quasi steady-state period during which both the emission rate and the transport and diffusion properties of the atmosphere remain fixed. The following sections describe the basic model concept as well as its application to multiple sources in an urban environment for both short- and long-term periods.

2.1 THE BASIC GAUSSIAN PLUME CONCEPT

Experimental data describing the distribution of concentration in plumes from point sources show that, although wide variations occur, these plumes exhibit a strong tendency toward a Gaussian or normal distribution as a statistical average (Pasquill 1962). To describe this distribution, consider a period of time with a constant point source emission rate of Q (units of mass per unit time) and a constant (in the horizontal plane) mean wind velocity (with magnitude u). In a standard three dimensional coordinate system with the origin beneath the point source which is at a height h above the ground, the x axis oriented in the direction of the mean wind, the y axis oriented normal to the mean wind deviation, and the z axis oriented vertically upwards, the ground-level concentration χ is

$$\chi = \frac{Q}{\pi u \sigma_y \sigma_z} \exp \left\{ -\frac{1}{2} \left(\frac{y^2}{\sigma_y^2} \right) + \frac{h^2}{\sigma_z^2} \right\} \qquad (1)$$

where

$$\sigma_y{}^2 = \frac{\int_{-\infty}^{\infty} y^2 \chi \, dy}{\int_{-\infty}^{\infty} \chi \, dy} \tag{2}$$

$$\sigma_z{}^2 = \frac{\int_{0}^{\infty} z^2 \chi \, dz}{\int_{0}^{\infty} \chi \, dz} \tag{3}$$

This relationship satisfies the continuity condition

$$\int_0^{\infty} \int_{-\infty}^{\infty} u \chi \, dy \, dz = Q. \tag{4}$$

The parameters σ_y and σ_z define the horizontal and vertical dimensions, respectively, of the pollutant cloud in a vertical plane perpendicular to the mean wind velocity. Estimates of σ_y and σ_z as functions of "alongwind" distance from the source give a complete specification of the concentration distribution.

Certain modifications have been introduced in the above equation to account for more realistic boundary conditions. In particular, one such modification is concerned with the marked reduction in vertical diffusion which is caused by a stable layer aloft, in addition to an impervious ground surface. Two techniques commonly employed to account for the effects of these boundaries were recently summarized by Calder (1970b). Another simple approximation which avoids the use of an infinite series in the solution was developed by Pasquill (1962). At some distance downwind, continued "reflection" of pollutants between the effective mixing ceiling and the ground surface will eventually lead to a uniform vertical distribution. Further reductions in pollutant concentrations will then be due only to crosswind diffusion. Pasquill suggested that the uniform vertical distribution will be approximately achieved at a downwind distance from the source at which σ_z is equal to the height of the effective mixing ceiling. He also suggested that out to a distance at which σ_z is equal to half this ceiling no effect due to "reflection" needs to be considered. If σ_z is represented as a simple power law of x, the following equations follow from these rules:

$$x_1 = \left(\frac{L}{2b}\right)^{\frac{1}{q}}, \quad x_2 = \left(\frac{L}{b}\right)^{\frac{1}{q}} \tag{5}$$

$$\sigma_z(x) = bx^q, \quad x \leq x_1 \tag{6}$$

$$\sigma_z(x) = \left(\frac{x + x_2 - 2x_1}{x_2 - x_1}\right) \frac{L}{2}, \quad x_1 \leq x \leq x_2 \tag{7}$$

$$\sigma_z(x) = L, \quad x \geq x_2 \tag{8}$$

where

x_1 = distance from source at which $\sigma_z(x) = L/2$,
x_2 = distance from source at which $\sigma_z(x) = L$,
L = vertical mixing ceiling,
$\sigma_z(x)$ = vertical diffusion parameter,
x = downwind distance from source, and
b, q = empirical constants.

It may be noted that this approach provides a simple method of using the σ_z concept for all travel distances from a source, and avoids the necessity of changing the diffusion model formulation at critical distances. This approach has been employed in this study.

The continuity condition assumed above may be modified by an exponential decay factor to account for various pollutant removal processes in the atmosphere. With a pollutant half-life of t_{50} and a decay time of x/u, equation (1) with the decay factor included becomes:

$$\chi = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left\{-\frac{y^2}{2\sigma_y^2} - \frac{0.693x}{t_{50}u} - \frac{h^2}{2\sigma_z^2}\right\} \qquad (9)$$

where

χ = concentration (mass/unit volume)

Q = source emission rate (mass/unit time)

u = mean wind speed (distance/unit time)

σ_y = standard deviation of the horizontal displacement of pollutants in the crosswind direction (distance)

σ_z = standard deviation of the vertical displacement of pollutants (distance)

x = horizontal coordinate in mean wind direction (distance)

y = horizontal coordinate in crosswind direction (distance)

z = vertical coordinate (distance)

t_{50} = pollutant half-life (time)

h = effective height of the source (distance)

0.693 = natural logarithm of 2

The effective height of the source is the sum of the physical release height and the plume rise due to its upward momentum and thermal buoyancy. The mean wind speed employed in the model should account for the known increase in wind speed with height above the ground. Some investigators have chosen to define this wind as that occurring at the physical stack height of the heated source (e.g., Smith 1968; Fortak 1969). Calder (1970) suggests the use of the wind speed at the estimated effective source height. Either of these choices is preferable to the use of an observed surface wind. In this study the wind speed at the effective source height is used.

2.2 ADAPTATION OF THE BASIC MODEL TO A PROTOTYPE SHORT-TERM MULTIPLE SOURCE MODEL

The basic Gaussian plume model describes the concentration field from a single point source during a short-term (i.e., steady-state) period. However, in an urban environment it is often necessary to consider emissions from many small sources (e.g., residential heating units), in numbers too large to treat each source individually. As a practical matter, individual large sources whose emission rates are significantly greater than other sources in the general vicinity are treated as point sources. The remaining emissions are treated as an area source whose emission rate and effective height are specified as a function of horizontal position using appropriate emission inventory techniques. As recently described by Calder (1970a), it is a simple matter to adapt the point source model to an area source. First, consider a reorientation of the coordinate system so that the origin is at a receptor point of interest and the x axis is pointed upwind into the mean wind direction. In this coordinate system, equation (9) gives the concentration at the receptor from a point source with horizontal coordinates (x, y).

Let q dx dy be the total amount of pollutant emitted per unit time in a horizontal element of area dx dy. Assuming that the total concentration at a receptor is the sum of concentration contributions from all individual area source elements, the concentration, χ_A, at the receptor location due to the area source is:

$$\chi_A = \int_0^{x_1} \int_{y_1}^{y_2} \frac{q(x, y)}{\pi u(h_A) \sigma_y(x) \sigma_z(x)} \exp\left\{ - \frac{y^2}{2\sigma_y^2(x)} - \frac{h_A^2}{2\sigma_z^2(x)} - \frac{0.693x}{t_{50} u(h_A)} \right\} dy\, dx \qquad (10)$$

where

h_A = effective area source emission height,

$q(x, y)$ = area source emission rate per unit area,

x_1 = distance to most upwind portion of emission area, and

y_1, y_2 = distances to furthermost crosswind portions of emission area.

The effect of these two types of sources (area and point) are analyzed separately and added together to give a resultant concentration.

The concentration χ_p at a receptor point due to N point sources is given by:

$$\chi_p = \sum_{i=1}^{N} \left[\frac{Q_i}{\pi u(h_i)\sigma_y(x_i)\sigma_z(x_i)} \exp \left\{ - \frac{y_i^2}{2\sigma_y^2(x_i)} - \frac{0.693\, x_i}{t_{50} u(h_i)} - \frac{h_i^2}{2\sigma_z^2(x_i)} \right\} \right] \quad (11)$$

where

the subscript i denotes values for the ith point source.

Equations (10) and (11) give the concentrations from area and point sources in an urban area during a single quasi steady-state period. The total concentration is given as the sum of that from the area and the point sources.

The use of the Gaussian plume model to represent concentrations from multiple sources in an urban environment has been studied by many investigators over the past decade. These efforts have resulted in the use of various techniques for simulation of the calculations required. A summary of some of these efforts and the results obtained are given in Appendix A.

Although the above equations provide the basis for applying the Gaussian plume model to an urban environment, the practical problem of defining appropriate parameter values still remains. Furthermore, since the model applies to a single steady-state period, it is necessary to define a period during which the model parameters are essentially constant. A steady-state period of one hour was adopted in this study for two reasons:

(1) Meteorological data is generally reported hourly.

(2) The parameter values used in the model should be representative of the short travel times which characterize the transport and diffusion of emissions from sources near a receptor.

The problem of defining parameter values is treated in Section 2.4.

2.3 LONG-TERM MODEL

The basic model described in Section 2.2 defines the urban concentration field for a single quasi steady-state period. However, mean concentrations over long-term periods during which both emission and meteorological conditions are significantly variable are also of interest. The short-term model is used to estimate long-term concentrations by assuming that the long-term period may be resolved into a succession of short-term quasi steady-state periods. This assumption is basic in the long-term models which have been developed by various investigators.

A straightforward application of this assumption was used by Turner (1964) to compute 24-hour mean concentrations. He divided 24-hour periods into a succession of 2-hour steady-state periods and obtained representative mean values of the model inputs for each 2-hour period. The 24-hour concentrations were then computed as the mean of the 2-hour period concentrations.

This approach represents a significant computational burden when used to obtain annual concentration means due to the large number of repetitions required. One possible alternative is to divide each model input into an exhaustive set of mutually exclusive categories and to determine the joint frequency distribution for the occurrence of all possible combinations of these categories. This is practical when the number of variable inputs is small and the number of categories for each variable is small. If one is only interested in the mean concentration over the period, and not concerned with the distribution of concentrations which occur, the assumption is commonly made in other studies that the model emission characteristics are independent of the meteorological characteristics (wind speed, wind direction and stability), and that they can be represented by mean input values in computing a mean concentration. This approach has been used by Martin and Tikvart (1968), Calder (1970) and Martin (1970).

Although relationships between diurnal variations in emission rates and meteorological characteristics are difficult to establish with currently available data, there are reasons to believe that significant correlations exist. For instance, the marked diurnal variation in diffusive capability of the atmosphere is correlated with the variation in emissions associated with the diurnal cycle of business activity. Similarly, cold and windy weather, associated with strong emissions from fuel consumption for space heating, tend to be correlated with northerly wind directions.

There is a need to collect and study emission-rate data so that their relationship to meteorological data can be clearly established. Significant efforts of this sort have been reported by Turner (1968a; 1968b) and Argonne National Laboratory (Croke and Roberts, 1971). Results from these studies have been utilized in this study to estimate hourly variations in emission rates using hourly temperature observations and the hour of the day.

The evidence of correlation between emission and meteorological parameters favors the use of the mean of the hour-to-hour sequence of concentrations over the mean determined from the joint frequency distribution of meteorological conditions.

One method of reducing the calculations required to estimate long-term mean concentrations is by statistical sampling of the quasi steady-state periods which make up the long-term period. Concentrations calculated for the selected periods are averaged to obtain the long-term mean concentration. The calculations may also be used to approximate the frequency distribution of short-term concentrations over the long-term period, by ordering the concentrations from lowest to highest value. This approach was applied in this study with considerable success (see Section 4.3.2). It is shown that statistical sampling can reduce the calculations required for seasonal concentrations by 90 percent or more.

2.4 MODEL PARAMETERS

The model described in Section 2.2 contains eight parameters which vary in time, space, or both. A discussion of available data and methods for assigning values to these parameters follows. The eight parameters are:

- Pollutant emission rate
- Plume rise
- Wind speed
- Wind direction

- Crosswind diffusion parameter
- Vertical diffusion parameter
- Vertical mixing ceiling
- Half-life for the decay of the pollutant with travel time.

In each case covered in our validation study (Section 4.0), we have selected the parametric option which we felt had the strongest and most objective support. The sensitivity analysis (Section 5.0) examines the impact of making other selections.

2.4.1 Emission Rates

Source emission rates vary both in time and space over an urban area. Spatial and temporal variations must be input for any pollutant whose field of concentrations is to be represented by the model. The level of detail to which these variations must be known is of particular concern in this study. The model, as described above, treats emission rates as uniformly representative of a general area (area source) or a particular location (point source). The definition of a significantly high emission rate, and the definition of the amount of change in emission rates over distance and time which is significant, are repeatedly considered in this study due to their impact on computational procedures, on model validation analysis, and on model sensitivity. These definitions also are important in determining the amount of effort that should be put into emission inventory surveys.

In general, emission rate estimates have been derived from a variety of information. Some available information is directly related to the sources (e.g., hourly megawatt loads on utility generator units, industrial production rates of emission generating processes, and the numbers of each type of residential fuel user in a standard metropolitan census area), while other information is related to emission rates by indirect reasoning (e.g., relationship of fuel consumption rate to ambient outside air temperature or to industrial plant work schedules). The following items are commonly used in estimating emission rates:

- City planning and zoning commission land maps
- Census bureau dwelling unit fuel use data
- Compilation of location, size, and nature of manufacturers, commercial operators, institutions, and apartments
- Emission inventory questionnaires and/or interviews
- Market data from fuel associations and fuel distributors
- Compiled emission factors (e.g., Ozolins and Smith, 1966)
- Production records of electric power companies and industrial plants.

An informative guide on problems and suggested solutions for collecting and analyzing emission inventory data has been written by Ozolins and Smith (1966). More detailed suggestions for analyzing the diurnal and weekly variations in emissions related to space heating requirements and to electric power plant operations have been made by Turner (1968a; 1968b). Another approach to modeling diurnal, weekly, and seasonal variations in emission rates which builds on Turner's suggestions has been reported by Roberts et al. (1970).

For the Gaussian plume model, as used in this study, it is considered appropriate to specify (based largely on Turner's and Roberts' work) the average emission rate for each representative area (e.g., a square mile) of the urban region for each period of the day (e.g., an hour). An individual source with an emission rate significantly higher than the average rate is specified separately as a point source.

In order to specify emission rates with high accuracy, it may be necessary to measure the emission characteristics of every individual source. However, there are clearly similarities among sources which allow them to be treated as neighborhoods, at least. For example, the size, spacing, and nature of urban buildings tend to be uniform, as evidenced by the existence of high-rise apartment neighborhoods, industrial areas, shopping centers, and low-rise housing developments. Furthermore, the similarity and consistency in people's habits and daily routines lead to predictability in the pattern of fuel usage by residential, commercial, or industrial facilities. Two methods of parameterizing the diurnal variations in SO_2 emissions and relating these variations to spatial variations have been used in this study: one for St. Louis (Turner 1968b), and one for Chicago (Roberts, et al., 1970). These are described more fully in Appendices B and C.

Criteria for setting the level of detail in space and time which should be reflected in emission data have not yet been defined. Some suggestions have been made for collecting data and for parameterizing emission information in general terms (e.g., a janitor function to represent diurnal stoking of residential furnaces, and empirical temperature-oriented corrections to account for commercial and residential diurnal fuel use). The question of more firmly settling this problem is addressed in the sensitivity portion of this study.

2.4.2 Plume Rise

It is characteristic that emissions from the larger sources are released from a tall stack in order to reduce their polluting effect in the immediate vicinity and in the nearby downwind area. In general, these emissions must also be hot and fast-moving for the stack to discharge its effluents adequately. As a result, they leave the stack with a considerable amount of upward momentum and thermal buoyancy. The effluent gases are accelerated upward; however, the upward momentum is continually diluted due to turbulent mixing with the ambient air. The resulting effect is a general leveling off of the effluent plume at some distance downwind.

Several formulas have been developed to predict the plume rise effect. A comprehensive review of these formulas and available plume rise observations by Briggs (1969) resulted in a set of recommended formulas which are simplifications and combinations of previous findings. The following recommended formulas are obtained from his conclusions:

$$\text{Let } h = h_s + \Delta h \qquad (12)$$

where

h = effective stack height

h_s = physical stack height

Δh = plume rise.

For all conditions:

$$\Delta h = 1.6 \frac{F^{0.33} x^{0.67}}{u}, \; x \le x_1 \tag{13}$$

For neutral and unstable meteorological conditions:

$$x_1 = 2.16 \; F^{0.4} h_s^{\;0.6}, \; h_s \le 305\text{m}$$

$$x_1 = 67.3 \; F^{0.4}, \; h_s > 305\text{m}$$

$$\Delta h = 1.6 \frac{F^{0.33} x_1^{\;0.67} \left\{ 0.4 + 0.64\left(\frac{x}{x_1}\right) + 2.2\left(\frac{x}{x_1}\right)^2 \right\}}{u\left[1 + 0.8\left(\frac{x}{x_1}\right)\right]^2}, \; x > x_1 \tag{14}$$

For stable meteorological conditions:

$$\left.\begin{aligned} x_1 &= \frac{2.4\;u}{\sqrt{s}} \\ \Delta h &= 2.9\left(\frac{F}{us}\right)^{0.33}, \; x > x_1 \end{aligned}\right\} \tag{15}$$

In the above equations,

$$F = \frac{gR}{\pi c_p p} Q_H \tag{16}$$

For standard pressure of one atmosphere,

$$\left.\begin{aligned} F &= 3.7 \times 10^{-5} Q_H \\ s &= \frac{g}{T} \left(\frac{\partial \theta}{\partial z}\right) \end{aligned}\right\} \quad (17)$$

where

F = buoyancy flux parameter, m^4/sec^3,

Q_H = heat emission due to efflux of stack gasses, cal/sec,

g = gravitational acceleration,

R = gas constant for air,

c_p = specific heat of air at constanct pressure,

p = atmospheric pressure,

T = average absolute temperature of ambient air, and

θ = average potential temperature of ambient air.

More detailed treatment of the special problem of inversion penetration by plumes from sources with significant exit velocities is also available from Briggs.

Certain limitations in the use of these formulas were noted by Briggs. Due to the lack of adequate data, he suggests that Equation 14 be applied only to a distance of five times x_1. In flat and uniform terrain, he concludes that observed plume rise may deviate from Equation 14 by ± 10 percent; in the vicinity of substantial terrain steps or near a large body of water, the deviations may be ± 40 percent. He also concludes that x_1 may vary by ±20 percent on the average with corresponding variations in Δh. These findings relate to neutral stability conditions.

In unstable conditions, the deviations may be larger and occur somewhat irregularly; however, the data presented by Briggs are not adequate to quantify this. With regard to stable conditions, the data presented by Briggs suggest that deviations in the nondimensional rise (i.e., $\Delta h/(F/us)^{0.33}$) as large as ± 0.5 may occur. When compared with his recommended mean nondimensional plume rise of 2.9, this deviation shows that deviations of ± 17 percent from Equation 15 have been observed in the developmental data.

In view of the dependence on downwind distance in the above plume rise equations, the following approximations from Briggs, without this dependence, for neutral and unstable conditions, are also of interest: For heat emission of 20 megawatts or more,

$$\Delta h = 1.6 \frac{F^{0.33}(10h_s)^{0.67}}{u}, \quad x \geq 10h_s \tag{18}$$

For other sources,

$$\Delta h = 1.6 \frac{F^{0.33}(3x_1)^{0.67}}{u}, \quad x \geq 3x_1 \tag{19}$$

Also, in the absence of wind and in primarily stable conditions,

$$\Delta h = 5.0 \frac{F^{0.25}}{s^{0.375}} \tag{20}$$

2.4.3 Wind Speed and Direction

The model hypothesizes the existence of a mean wind speed and direction; therefore, data must be obtained which are suitable for defining these means. In many urban areas, wind monitoring equipment is installed simultaneously with air quality monitoring equipment. As a result it is frequently possible to consider wind observations from several representative points which can be vectorially averaged to obtain a mean wind direction and speed. However, it is often necessary to use a single airport observation to define the wind direction and speed.

Since wind speeds near ground level under certain conditions show considerable increase with height, it is desirable to account for the increased transport speed associated with emissions from sources with large effective heights. However, it is difficult to decide on a height which is appropriate for defining the transport.

The wind profile may be represented empirically in the lowest layers of the atmosphere by a power law (e.g., Munn, 1966). An extensive summary of such power laws observed on a 125-meter tower at Brookhaven National Laboratory were reported by DeMarrais (1959). Let

$$u(z) = u_1 \left(\frac{z}{z_1}\right)^a \tag{21}$$

where

$u(z)$ = wind speed at height z,

u_1 = wind speed at reference height z_1,

a = empirical wind profile parameter.

When vertical wind observations are available from a tower, the parameter (a), along with values for z_1 and u_1, may be determined directly. When tower data are not available, estimates of (a) must be deduced indirectly. DeMarrais (1959) concluded that (a) ranges between 0.1 and 0.3 during the day and between 0.2 and 0.8 at night. From data presented by Munn (1966) there is also a clear correlation of (a) with time of day which is consistent with DeMarrais' findings. A recent study of wind profiles in New York City (Singer et al., 1970) suggests that the extreme roughness of that city's terrain is so dominating that for winds up to 900 feet there is very little variation from day to day or from day to night about a mean value of 0.10 for (a).

The data used in the validation and sensitivity studies are from Chicago and St. Louis. In the absence of other information, the results regarding (a) observed for New York City are applied to Chicago for unstable conditions. For other stability conditions and for St. Louis for all stability conditions, values intermediate between those found in New York City and the more extensive rural values are considered appropriate.

2.4.4 Diffusion Parameters

A large number of empirical functions have been proposed by investigators to represent the diffusion parameters σ_y and σ_z. In each set of σ_y and σ_z parameters, the values vary with the stability of the atmospheric boundary layer. Three sets of diffusion parameter values (one from Pasquill, 1962, and two from McElroy and Pooler, 1968) and the associated meteorological parameters used to characterize stability are discussed below.

The most widely used functions for σ_y and σ_z are based on diffusion estimates originally proposed by Pasquill in a form presented by Gifford (1961). A convenient graphical presentation of these functions is given by Turner (1969) who indicates that these values are representative for a sampling time of minutes to hours and apply strictly to open, level terrain. Turner further notes that these values are probably too small for low-level pollutant release in urban areas. The principal basis for this conclusion is shown in a recent study published by McElroy (1969). These functions (Pasquill, 1962) are widely employed values for σ_y and σ_z in air pollution analysis.

The graphical representations of the Pasquill diffusion parameters (e.g., Turner, 1970) have been approximated in this study by power law functions. For σ_y values, a single power law, 0.903, was found to be appropriate over all for the five stability classes commonly used in urban diffusion analysis. These classes correspond to categories A to E in Gifford's presentation. The fitted curves (indistinguishable from the original graphs) are shown in Figure 1. Values for the fitted constant (a) in the following relationship are listed in Table 1.

$$\sigma_y = ax^{0.903} \tag{22}$$

The Pasquill σ_z parameter curves do not occur as simple power functions, but they were closely approximated by the piecewise power functions shown in Figure 2. The selected intervals and the appropriate fitted constants for each interval are also listed in Table 1.

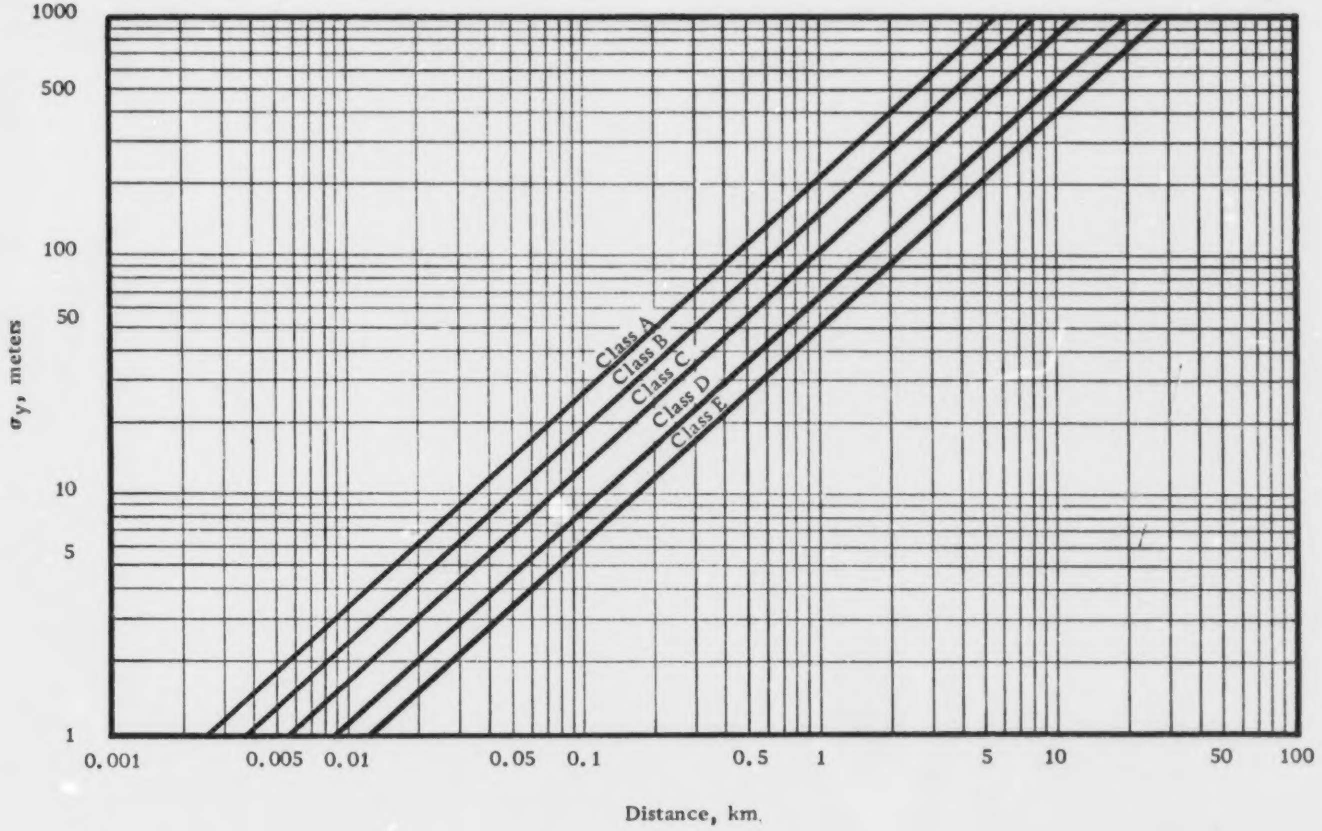


Figure 1. Pasquill σ_y Diffusion Parameter as a Function of Distance Downwind and Stability Class

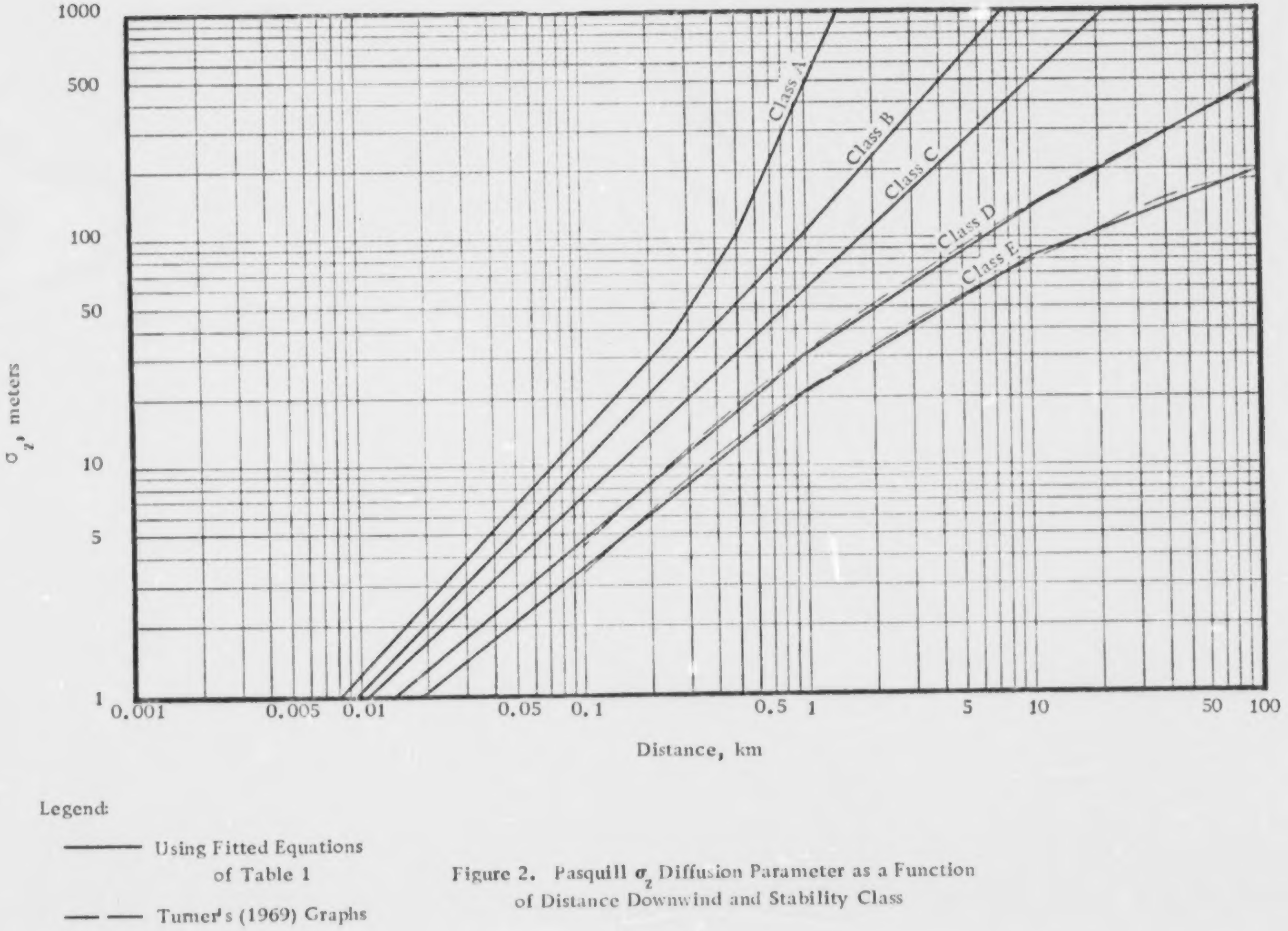


Figure 2. Pasquill σ_z Diffusion Parameter as a Function of Distance Downwind and Stability Class

Table 1. Fitted Constants for the Pasquill Diffusion Parameters

Stability Class	Crosswind Constant(1) a	Constants for Vertical Diffusion Parameter, σ_z(2)							
		$x \leq x_1$		x_1	$x_1 \leq x \leq x_2$		x_2	$x_2 \leq x$	
		b	q	(Meters)	b	q	(Meters)	b	q
A	0.40	0.125	1.03	250	0.00883	1.51	500	0.000226	2.10
B	0.295	0.119	0.986	1000	0.0579	1.09	10,000	0.0579	1.09
C	0.20	0.111	0.911	1000	0.111	0.911	10,000	0.111	0.911
D	0.13	0.105	0.827	1000	0.392	0.636	10,000	0.948	0.540
E	0.098	0.100	0.778	1000	0.373	0.587	10,000	2.85	0.366

(1) $\sigma_y = ax^{0.903}$, Where x isDownwind Distance from Source; σ_y and x are in Meters.

(2) $\sigma_z = bx^q$; σ_z and x are in Meters.

Among other empirical functions for σ_z developed from field trial observations are those reported by Singer and Smith (1966), Cramer (1964), Milly (1958), and Hilst and Bowne (1966). These investigators have characterized reported results into a system of functions which are related to a range of atmospheric stability conditions. Empirical functions for σ_y have been developed by Singer and Smith (1966), Cramer (1964), Islitzer (1961), and Fuquay, Simpson, and Hinds (1964). All of these investigators except Hilst and Bowne developed their results from experiments conducted in relatively open terrain, remote from urban influences. Furthermore, the values reported by Milly, and Hilst and Bowne, are for instantaneous as opposed to continuous sources. Thus, none of the above sets of diffusion parameters are completely relevant to the applications of concern in this study, namely, air pollution diffusion in urban terrain from continuous sources. The information most relevant to diffusion parameter values in an urban environment is that provided by McElroy and Pooler (1968). Their study characterized observed values of σ_y and σ_z from continuous tracer emissions in the city of St. Louis according to several systems of meteorological stability classification. The question of the proper system of stability classification has not been satisfactorily resolved; however, certain observations regarding this problem may be noted.

Meteorological stability measures are used to stratify observed diffusion parameters (σ_y and σ_z) and, in model applications, to differentiate steady states. These measures have varied from the subjective estimates of insolation (used by Pasquill to characterize daytime stability) to detailed measures of turbulence (such as the wind speed trace used by Singer and Smith, or the standard deviation in wind direction used by Hay and Pasquill (1957), Cramer (1964), and Islitzer (1961)). The validity and usefulness of these different measures are matters requiring further study. A completely objective system of meteorological stability classifications which is widely employed with the classes of diffusion parameters defined by Pasquill was suggested by Turner (1964). This system is described in Tables 2 and 3 and has been used in this

Table 2. Meteorological Stability Classifications for Characterizing the Diffusion Parameters (σ_y and σ_x)

Wind Speed (Knots)	Stability Class for Indicated Net Radiation Index *						
	4	3	2	1	0	-1	-2
0, 1	A	A	B	C	D	E	E
2, 3	A	B	B	C	D	E	E
4, 5	A	B	C	D	D	E	E
6	B	B	C	D	D	E	E
7	B	B	C	D	D	D	E
8, 9	B	C	C	D	D	D	E
10	C	C	D	D	D	D	E
11	C	C	D	D	D	D	D
≥12	C	D	D	D	D	D	D

*Net Radiation Index Values are Given in Table 3.

Table 3. Net Radiation Index Values

Time of Day	Total Cloud Amount (t)	Ceiling (c), (ft)	Net Radiation Index for Indicated Solar Altitude (a)			
			$a \leq 15^\circ$	$15^\circ \leq a \leq 35^\circ$	$35^\circ \leq a \leq 60^\circ$	$a > 60^\circ$
Night	$t \leq 0.4$	--	-2	--	--	--
Night	$0.4 < t < 1.0$	--	-1	--	--	--
Night	$t = 1.0$	$c < 7{,}000$	0	--	--	--
Night	$t = 1.0$	$c \geq 7{,}000$	-1	--	--	--
Day	$t < 1.0$	$c \geq 16{,}000$	1	2	3	4
Day	$0.5 < t < 1.0$	$c < 7{,}000$	1	1	1	2
Day	$0.5 < t < 1.0$	$16{,}000 > c \leq 7{,}000$	1	1	2	3
Day	$t = 1.0$	$c \leq 7{,}000$	0	0	0	0
Day	$t = 1.0$	$16{,}000 > c \geq 7{,}000$	1	1	1	2
Day	$t = 1.0$	$c \geq 16{,}000$	1	1	2	3

study. The solar altitude (e.g., Sutton, 1953) required in this system may be computed by the following formula (expressed in arctan rather than arcsin form):

$$\alpha = \arctan\left\{\frac{\sin\phi\sin\delta + \cos\phi\cos\delta\cos\left[\frac{\pi}{12}(h-12)\right]}{\sqrt{1 - \left\{\sin\phi\sin\delta + \cos\phi\cos\delta\cos\left[\frac{\pi}{12}(h-12)\right]\right\}^2}}\right\} \tag{23}$$

$$\delta - 23.5\left(\frac{\pi}{180}\right)\sin\left\{\frac{\pi}{180}\left[30(m-1) + d-80\right]\right\}$$

where

α = solar altitude

δ = solar declination

m = month of year

d = day of month

h = hour of day

ϕ = latitude.

Recently a new objective system for classifying the Pasquill stability categories was suggested by Ludwig et al. (1970). This scheme relates more directly to Pasquill's initial guidelines by using the following definitions of insolation (I) classes:

Slight $\equiv I \leq 0.33$
Moderate $\equiv 0.33 < I \leq 0.67$
Strong $\equiv 0.67 < I$

where

$I = (1-0.5N)\ \mathrm{Sin}\,\alpha$

N = cloud cover (fraction of sky obscured)

α = solar altitude

Cloud layers reported as thin are ignored in determining N. With these definitions, Pasquill's original table, shown in Table 4, may be used. The table shown includes the original Pasquill categories except that his category F, and his two blank categories, have been designated as E, (following Turner's, 1964 concept) since moderately stable conditions rarely, if ever, exist in the urban environment. Also, the nighttime cloud cover categories have been modified slightly to accommodate cloud cover reports in tenths rather than eighths and to make them exhaustive as well as mutually exclusive. It may be noted that Pasquill recommended taking the average of two categories where dual classes are designated.

Table 4. Pasquill's Stability Categories for Diffusion Parameters

Surface Wind Speed at 10m (m/sec.)	Daytime Insolation			Night Cloud Cover (1)	
	Strong	Moderate	Slight(2)	Thinly Overcast or ≥0.5 Opaque(2)	<Overcast Thin or <0.5 Opaque
<2	A	A-B(3)	B	E	E
2 to<3	A-B(3)	B	C	E	E
3 to<5	B	B-C(3)	C	D	E
5 to 6	C	C-D(3)	D	D	D
>6	C	D	D	D	D

(1) Night Refers to Period One Hour Before Sunset to One Hour After Dawn.
(2) Use Class D for All Wind Speeds in Presence of Opaque Overcast.
(3) Use Average of the Two Classes.

The diffusion parameters presented by McElroy and Pooler (1968) are based on data that is representative of the influence of an urban environment. These authors stratified the experimental results by means of several classes of meteorological stability measures and estimated functional relationships between σ_y and σ_z and travel distance for each class. The relationships presented graphically by McElroy and Pooler have been fitted to power laws in this study.

The curves have been extrapolated from 600 to 10 meters as shown in Figures 3 through 6. The fitted equations have the forms,

$$\sigma_y = ax^p \qquad\qquad (24)$$

$$\sigma_z = bx^q$$

The values obtained for a, b, p, and q for two meteorological stability classes are given in Tables 5 and 6.

The values in Table 5 are classified in terms of (σ_θ) and the bulk Richardson number as defined by Lettau (1957). In the study used to classify the parameter values, the following equation was used (indicated numerical values refer to the St. Louis data used in the study).

$$Ri_B = \frac{g(\frac{\Delta T}{\Delta Z} + r_d)\ Z^2}{\bar{T}\ u^2} \qquad (25)$$

where

Ri_B = bulk Richardson number

ΔT = temperature at 140m less temperature at 39m

ΔZ = 140m - 39m = 101m

r_d = adiabatic lapse rate

Z = height of upper anemometer, 140m

$\bar{T}$ = mean absolute temperature for 39 to 140m layer

u = wind speed at height Z.

The values in Table 6 are presented for the Turner stability classes. Figures 3 through 6 also show the diffusion parameters for the two systems of stability classifications.

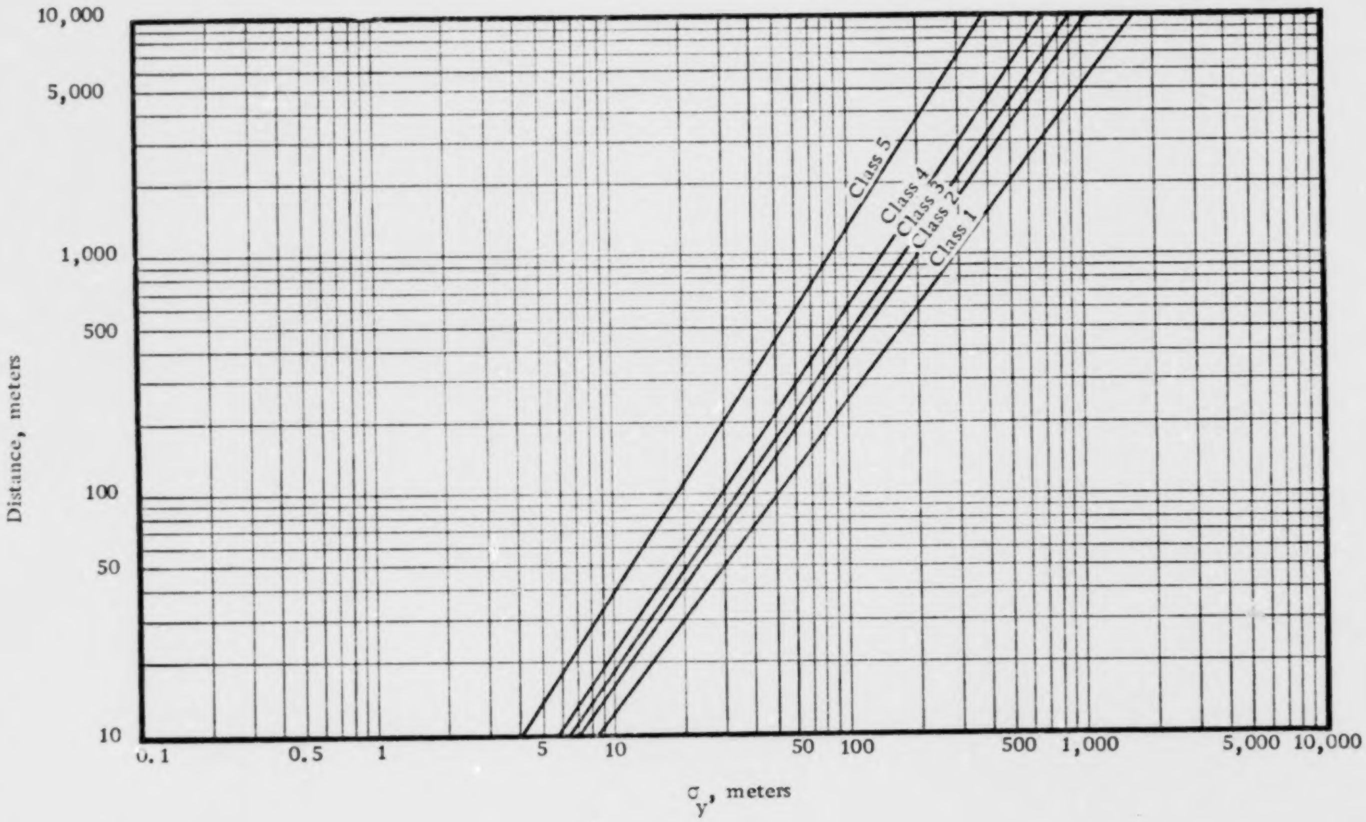


Figure 3. McElroy-Pooler σ_y Diffusion Parameter for Different Stability Classes Based on Bulk Richardson Number

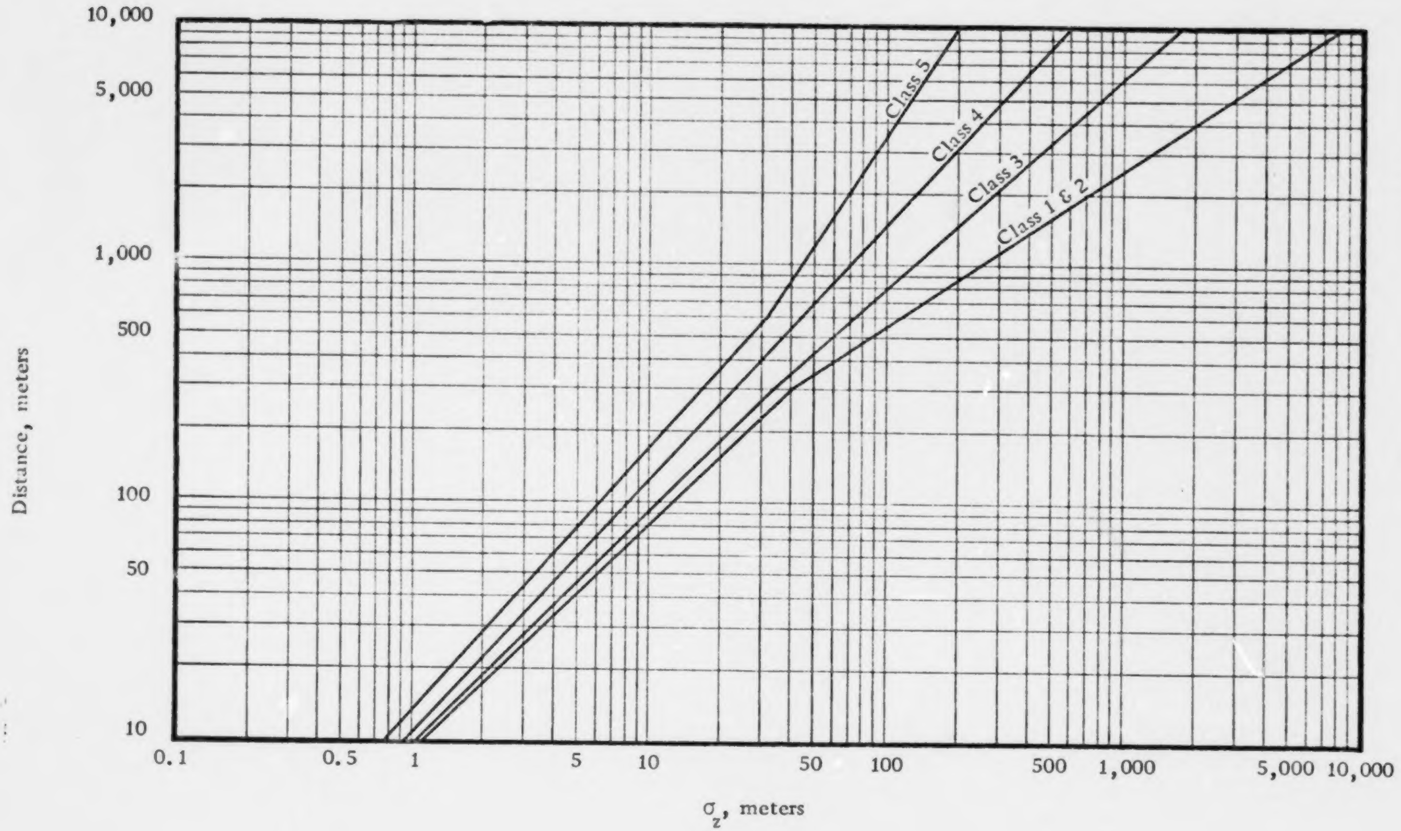


Figure 4. McElroy-Pooler σ_z Diffusion Parameter for Different Stability Classes Based on Bulk Richardson Number

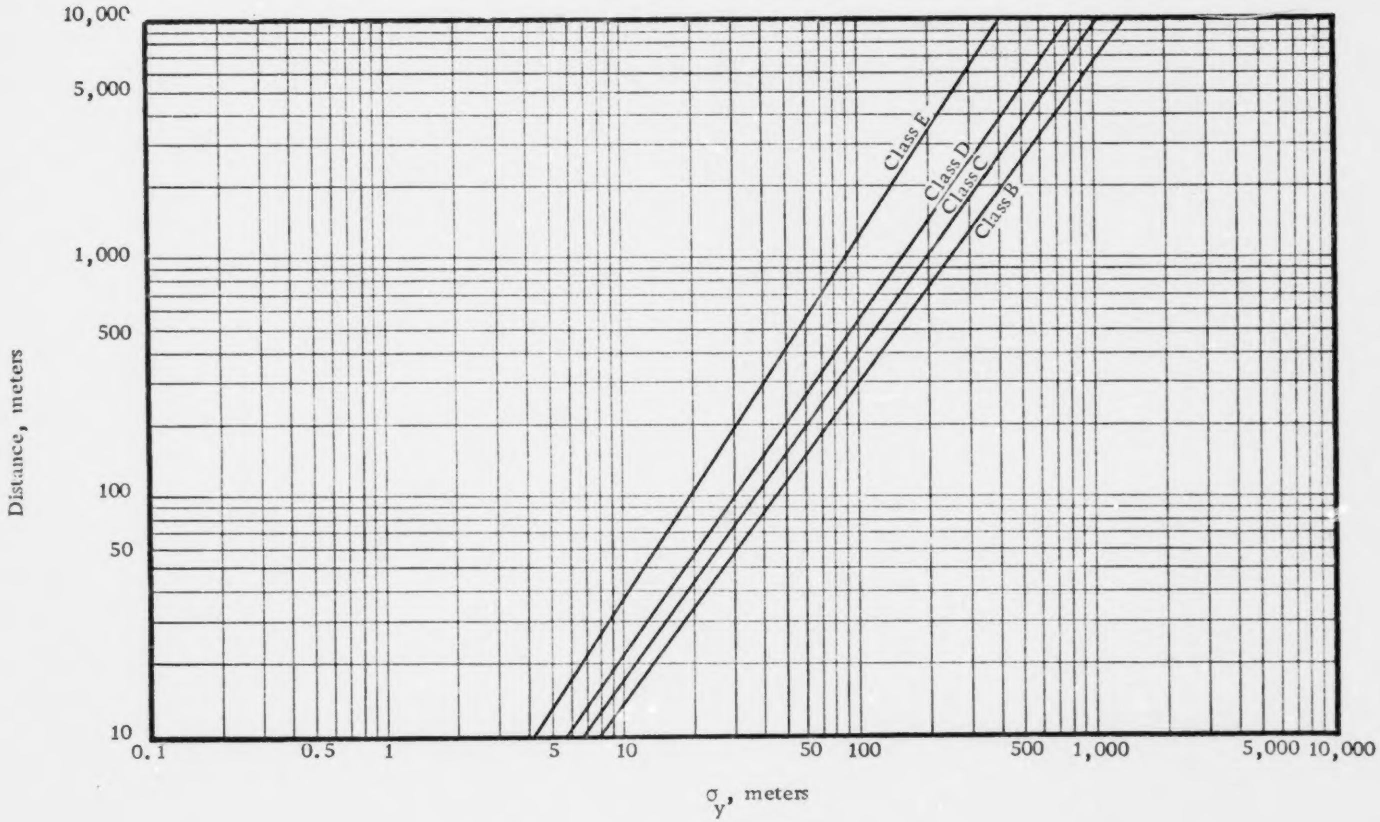


Figure 5. McElroy-Pooler σ_y Diffusion Parameter for Different Stability Classes Based on Turner Stability Index

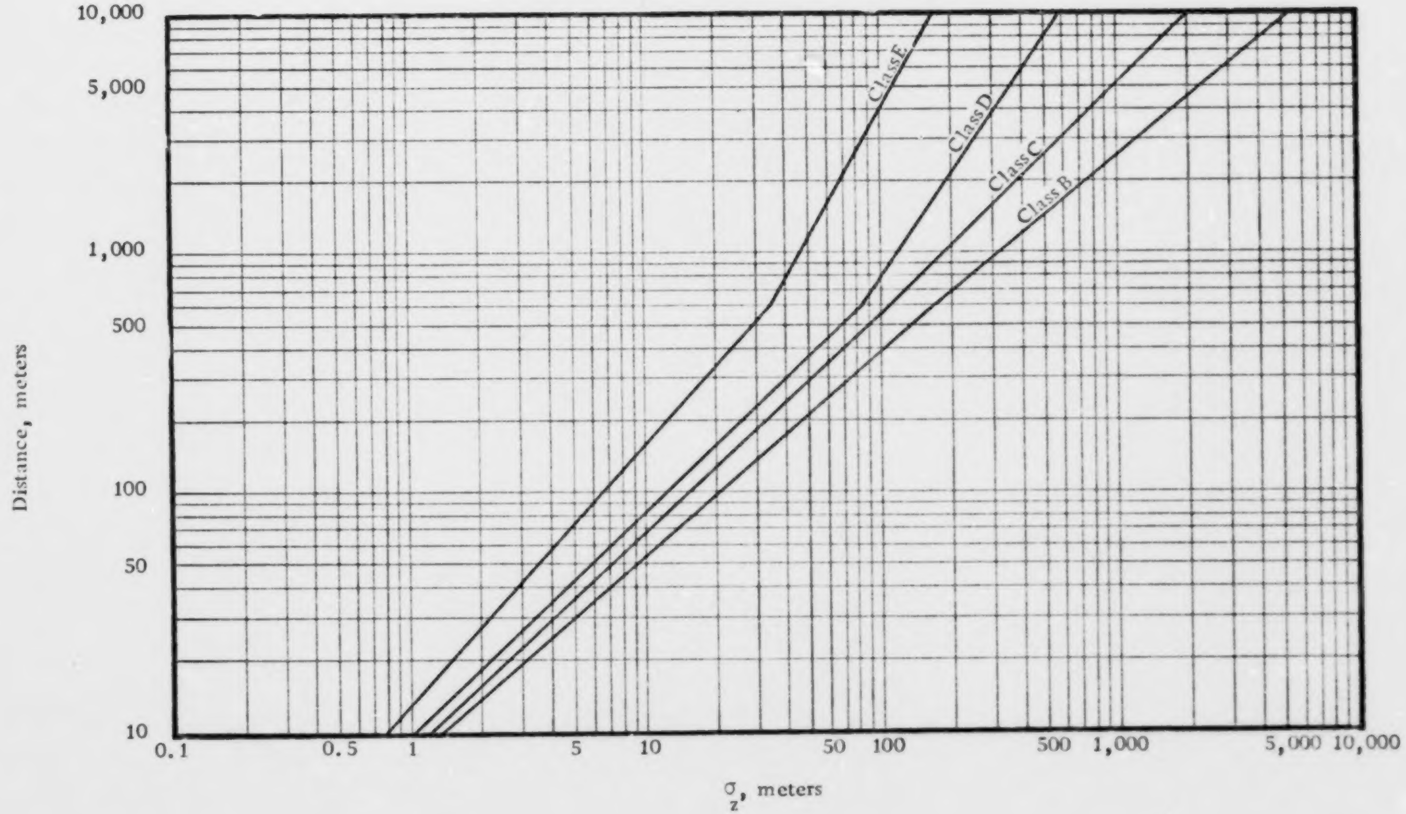


Figure 6. McElroy-Pooler σ_z Diffusion Parameter for Different Stability Classes Based on Turner Stability Index

Table 5. Fitted Constants for the McElroy-Pooler Diffusion Parameters Based on σ_θ (1) and Ri_B (2) Stability Classifications

Stability Category			Crosswind Constants(3)		Constants for Vertical Diffusion Parameter(4)				
					$x \leq x_1$		x_1	$x \geq x_1$	
Index	σ_θ (Degrees)	Ri_B	a	p	b	q	(Meters)	b	q
1	>29.5	<-0.01	1.49	0.761	0.118	1.02	300	0.00724	1.51
2	23 to 29.5	<-0.01	1.40	0.719	0.118	1.02	300	0.00724	1.51
3	<23	<-0.01	1.26	0.712	0.115	1.00	300	0.0581	1.12
4	-	-0.01 to 0.01	1.14	0.698	0.110	0.934	600	0.110	0.934
5	-	>0.01	0.945	0.648	0.478	0.907	600	0.478	0.655

(1) Standard Deviation of Horizontal Wind Direction.

(2) Lettau's (1957) Bulk Richardson Number.

(3) $\sigma_y = ax^p$, Where x is Downwind Distance from Source; σ_y and x are in Meters.

(4) $\sigma_z = bx^q$; σ_z and x are in Meters.

Table 6. Fitted Constants for the McElroy-Pooler Diffusion Parameters Based on Turner Stability Classifications

Stability Index	Crosswind Constants (1)		Constants for Vertical Diffusion Parameter (2)			
			$x \leq 600$		$x \geq 600$	
	a	p	b	q	b	q
A	-	-(3)	-	-	-	-
B	1.42	0.745	0.0926	1.18	0.0720	1.22
C	1.26	0.730	0.0891	1.11	0.169	1.01
D	1.13	0.710	0.0835	1.08	1.07	0.682
E	0.992	0.650	0.0777	0.955	1.01	0.554

(1) $\sigma_y = ax^P$, Where x is Downwind Distance from Source; σ_y and x are in Meters.

(2) $\sigma_z = bx^P$; σ_z and z are in Meters.

(3) Not Available from McElroy and Pooler Data.

The atmospheric stability categories defined by σ_θ and Ri_B provide better stratification of σ_y and σ_z values determined from field experiments than do the Turner stability categories. However, it is required that vertical temperature observations be obtained from a tower and that turbulence statistics be obtained either from a suitably located bivane instrument or from statistical analysis of wind direction traces of conventional wind recorders. The Turner stability categories can be determined from routine airport weather observations. Thus, although the Turner stability classes may result in greater uncertainty regarding the true diffusive capability of the atmosphere at any given time, they may be preferable due to their greater availability. An alternative to using the McElroy-Pooler (1968) stability classes would be to use the Brookhaven wind gustiness classes (Singer and Smith, 1966). This alternative was pursued by McElroy and Pooler. However, their investigation led to redefining the meteorological characteristics of the classes and introducing new diffusion parameters to associate with each class. As a result, this approach leads to serious questions concerning the generality of this stability classification system. It should be noted that the generality of the McElroy-Pooler classifications also remains unproven until they can be verified at an independent site.

2.4.5 Vertical Mixing Ceiling

The vertical mixing ceiling is defined as that height above ground level at which there is a marked reduction in vertical diffusion. Such barriers are observed as a sharp drop in the concentration observed in a vertical sounding (e.g., Davidson, 1967). It may be observed as a delineation between the smoke-filled layer and cleaner air aloft over many cities in the early morning. Much higher ceilings typical of afternoon hours are clearly visible to air travelers in climbing to or descending from cruising altitudes. The ceiling may vary from 100 meters at night to over 1500 meters during the day. Hourly estimates of the ceiling are required for use in the model.

Unfortunately, this mixing ceiling is not always visibly discernible and no routine systems for taking vertical soundings of pollutant materials are in operation. Therefore, the ceiling is generally inferred from temperature soundings which are routinely observed twice daily at certain airports by the National Oceanic and Atmospheric Administration (NOAA). These observing locations are separated by about 200 km on the average and are usually located outside the urban area. The mixing layer is generally characterized by a near adiabatic lapse rate extending from the ground to some altitude at which a deep, (several kilometers) more stable lapse rate exists. However, the vertical temperature structure of the atmosphere is frequently not this well defined. As a result, considerable judgment may be required to define where, in a vertical temperature profile, an effective mixing ceiling exists. Unfortunately very little data have been collected on the relationship between vertical pollution and temperature profiles which could be used to develop and substantiate rules for defining the mixing ceiling over an urban region.

The procedure which is generally used to define the mixing ceiling is the following: Determine the general rural vertical temperature profile from the nearest appropriate (same air mass) radiosonde, or by interpolation of two or more nearby radiosondes. Estimate minimum morning and maximum afternoon air temperatures which are representative of the urban area. The afternoon temperature may be obtained directly from airport observations or other available data. In most cases the morning urban temperature will exceed the rural temperature. The following equation (Ludwig et al., 1970) may be used to estimate morning urban temperatures (T_u) from rural temperatures (T_r) using the urban population Φ and the radiosonde temperature lapse rate (dT/dp) as parameters:

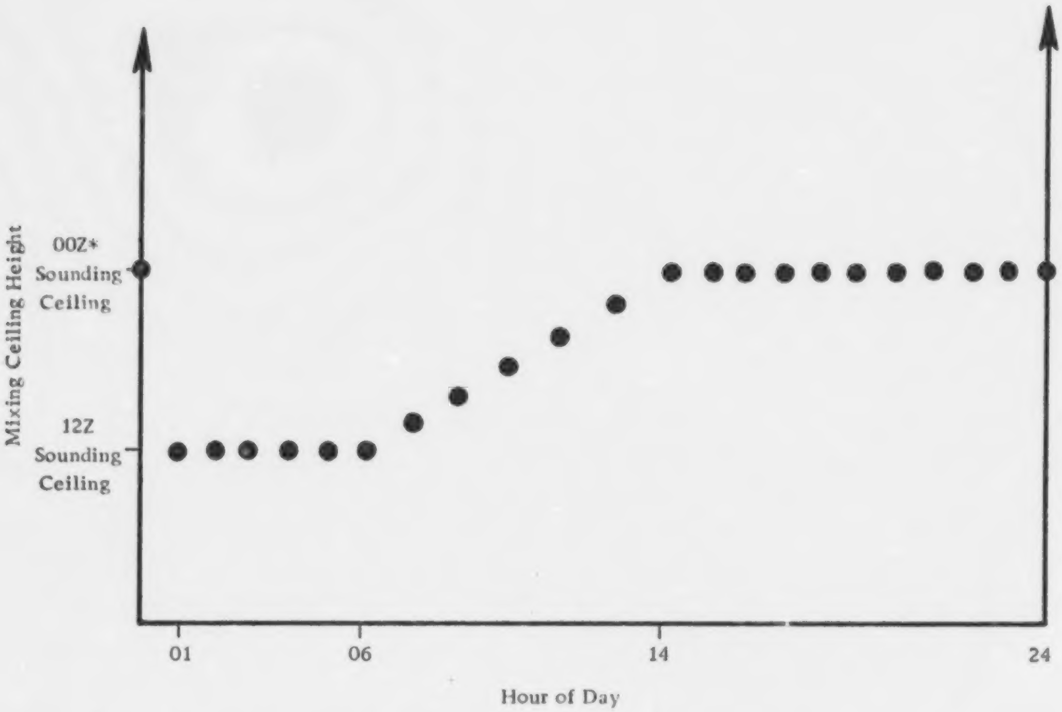
$$T_u = T_r + \Phi^{0.25}(0.0633 - 0.298 \frac{dT}{dp}) \qquad (26)$$

Construct adiabatic temperature profiles from the urban temperatures which intersect the rural temperature profile. The height of these intersections are assumed to be the minimum and maximum mixing ceilings. A method of interpolating between these values to give hourly estimates is to:

1. Use the morning minimum from midnight to 6 a.m.
2. Linearly interpolate between the minimum and the maximum between 6 a.m. and 2 p.m.
3. Use the afternoon maximum between 2 p.m. and midnight.

This pattern of diurnal variations is illustrated in Figure 7.

Limited simultaneous observations of temperature and SO_2 or particle concentration profiles reported by Davidson (1967),



*Z Means Greenwich Standard Time

Figure 7. Graphical Model of Procedure Used to Interpolate in Time Between Mixing Ceiling Estimates Obtained for Standard Radiosonde Observing Times

Roberts et al. (1970) and McCaldin and Sholtes (1970) attest to the general validity of this approach.

Several methods of implementing this approach and for interpolating between radiosonde observations both in space and time have been reported by Holzworth (1967), Roberts et al. (1970) and Ludwig et al. (1970). These investigators have also differed in the technique used to estimate representative urban temperatures which frequently are not recorded routinely. The choice among these details should most appropriately be governed by the nature of the data with which the model will be used.

2.4.6 Pollutant Decay

Atmosphere removal processes are approximated in the model by an exponential decay of the pollutant with travel time. The removal processes are parameterized by specifying a pollutant half-life. However, due to the limted data and the wide variety of removal processes which may be operating, it is difficult to define an appropriate half-life.

Information regarding SO_2 removal processes consists of atmospheric and laboratory experiments (reviewed by Urone and Schroeder, 1969), comparisons of SO_2 concentrations with other materials in the atmosphere (e.g., Weber, 1970; 1970a and Manowitz et al., 1970), and less direct comparisons of observed SO_2 concentrations and other tracer materials with model computations.

The general conclusion drawn from this evidence in that the SO_2 half-life under various defined atmospheric conditions can range from ten's of minutes to several days, with several hours being a preferred range under many urban conditions (a nominal value of four hours has been used in many previous studies).

Our validation study which used SO_2 data for validation purposes assumed negligible decay. In the sensitivity analysis, the impact of various decay levels is assessed.

Section 3.0

MODEL IMPLEMENTATION

In this study a computer program was developed for the Gaussian plume, multiple-source urban diffusion model described in Section 2.0. The basic objective of this work was to find algorithms which are numerically accurate, computationally efficient, and appropriate to the spatial and temporal variations in inputs and outputs which were to be considered in the validation and sensitivity analyses. Particular attention was given to numerical integration algorithms and to the selection of appropriate parameter values for these algorithms.

The basic theory and format structure of the model employed were presented in the preceding sections. In this presentation, it was noted that emission inventory data for SO_2 sources are typically of two types: one includes significant point sources such as power plant stacks, large industrial plants, and large commercial and municipal emitters; the other is related to the large number of less intense but widespread emitters such as residential homes, high-rise apartments, and various smaller commercial and industrial establishments. These are treated as area sources with one of three effective heights. The concentration at any receptor point may be estimated by computing the contribution from each of these two types of sources separately and adding the results. The equations used to perform these calculations are:

$$\chi = \chi_p + \chi_A \qquad (27)$$

$$\chi_p = \sum_{i=1}^{N} \frac{Q_i}{\pi u(h_i)\,\sigma_y(x_i)\,\sigma_z(x_i)} \exp\left\{-\frac{h_i^2}{2\sigma_z^2(x_i)} - \frac{y_i^2}{2\sigma_y^2(x_i)} - \frac{0.693\,x_i}{t_{50}\,u(h_i)}\right\} \qquad (28)$$

$$\chi_A = \sum_{i=1}^{3} \int_{y_1}^{y_2} \int_{0}^{x_1} \frac{q(x,y,h_i)}{\pi u(h_i)\,\sigma_y(x)\,\sigma_z(x)} \exp\left\{-\frac{h_i^2}{2\sigma_z^2(x)} - \frac{y^2}{2\sigma_y^2(x)} - \frac{0.693\,x}{t_{50}\,u(h_i)}\right\} dxdy \qquad (29)$$

where

N = number of point sources

Q_i = emission rate for ith point source

$q(x,y,h_i)$ = emission rate per unit area for height h_i

$u(h_i)$ = wind speed

h_i = effective source height

t_{50} = half-life of pollutant due to atmospheric removal processes

$\sigma_y(x), \sigma_z(x)$ = diffusion parameters.

The preceding equations use wind-oriented coordinates with the x-axis oriented into the mean wind direction and with the origin at a receptor location. However, it is more convenient to assign receptor and source coordinates relative to a fixed coordinate system denoted (ξ,η), with ξ denoting the east-west coordinate and η denoting the north-south coordinate. Equation 28 is applied to a particular receptor location (ξ_R,η_R) by using a coordinate transformation for the point source locations (ξ_i,η_i). For a given wind direction θ

(i.e., azimuth in degrees measured clockwise from north) the wind-oriented coordinates (x_i, y_i) are

$$x_i = (\xi_i - \xi_R) \sin \theta + (\eta_i - \eta_R) \cos \theta \tag{30}$$

$$y_i = (\eta_i - \eta_R) \sin \theta - (\xi_i - \xi_R) \cos \theta \tag{31}$$

When Equation 29 is applied to the particular receptor (ξ_R, η_R), numerical integration techniques require that the integrand be known for certain values of the integration variables x and y, which are wind-oriented coordinates. This requires that $q(x,y,h_i)$ be known for specified (x,y). Since q will be recorded in terms of the fixed coordinates (ξ,η) the following transformations are required to determine the ξ,η coordinates which correspond to selected (x,y) values.

$$\xi = \xi_R + x \sin \theta - y \cos \theta \tag{32}$$

$$\eta = \eta_R + x \cos \theta + y \sin \theta \tag{33}$$

3.1 NUMERICAL EVALUATION OF CONCENTRATIONS FROM AREA SOURCES

Numerical integration processes required to evaluate Equation 29 affect both the accuracy achieved and the cost expended in computation time. Therefore, the following three approaches in decreasing order of computational detail were considered for evaluating the double integral in Equation 29.

- Numerical evaluation of the double integral
- Use of the "virtual" point source concept

- Use of the "narrow plume" assumption to reduce the double integral to a single integral.

The first approach is a straightforward evaluation of the double integral by numerical techniques. One method of doing this is to divide the area source into small subdivisions $\Delta\xi$ by $\Delta\eta$. If the integrand (I_{ijk}) in Equation 29 is evaluated at the center of each subdivision (i.e., fixed-axis oriented coordinates ξ_i, η_j), the double integral may be approximated by a double summation.

$$\chi_A \approx \sum_{i=1}^{3} \Delta\xi \; \Delta\eta \sum_{j} \sum_{k} I_{ijk} \tag{34}$$

This is mathematically equivalent to replacing each subdivision of the area source by a point source with emission rate $q(\xi_j, \eta_k, h_i)\ \Delta\xi\ \Delta\eta$ at each emission height h_i. In an application of this approach, Fortak (1970) found that a suitable size for the subdivisions which would give a satisfactory approximation to the integral for a wide range of wind speeds and stability categories was 50 meters by 50 meters. In this study, the double integration has been carried out by repeated application of the trapezoid rule.

In the second approach to numerical integration, the initial vertical and horizontal distributions of concentration from pollutants emitted within a subdivision of the area source are approximated by a bivariate normal function. The double integration in Equation 29 is replaced by a summation of double integrals over each subdivision. Let σ_{ys} be the standard deviation of the initial horizontal distribution of concentration in a subdivision and σ_{zs} be the standard deviation of the initial vertical distribution of concentration in a subdivision. In terms of the diffusion parameter functions, $\sigma_y(x)$ and $\sigma_z(x)$ (e.g., see Figures 5 and 6), there is a downwind travel distance x_y which corresponds to σ_{ys} and a distance x_z which corresponds to σ_{zs}. This means that a point source located a distance x_y upwind of the center of the subdivision will produce the approximate horizontal crosswind distribution of initial concentrations from emissions within the subdivision area . A point source located a distance x_z upwind will produce the approximate vertical distribution. These "virtual" distances are used in the point source diffusion Equation 9 to define subsequent changes in the initial distribution of concentration. It is only necessary to replace $\sigma_y(x)$ and $\sigma_z(x)$ by $\sigma_y(x + x_y)$ and $\sigma_z(x + x_z)$ and to let Q be the total emission rate from the subdivision of the area source. Using this concept, the double integration over a subdivision of the area source is approximated by a "virtual point source," and the double integral of Equation 29 is replaced by the summation of the concentrations from all subdivisons.

$$\chi_A = \sum_{i=1}^{3} \sum_{j=1}^{J} \frac{q_j(h_i)\, A_j}{\pi u(h_i)\, \sigma_y(x_j+x_{y,j})\, \sigma_z(x_j+x_{z,j})} \exp\left\{- \frac{h_i^2}{2\sigma_z^2(x_j+x_{z,j})} - \frac{y_j^2}{2\sigma_y^2(x_j+x_{y,j})} - \frac{0.693\, x_j}{t_{50}\, u(h_i)}\right\} \quad (35)$$

where

J = number of area subdivisions

$q_j(h_i)$ = emission rate per unit area for jth subdivision at height h_i

A_j = area of jth subdivision

x_j = alongwind distance from the receptor to the center of the jth subdivision

y_j = crosswind distance from the receptor to the center of the jth subdivision

$x_{y,j}$ = "horizontal" virtual distance, i.e., $\sigma_y(x_{y,j}) = (\sigma_{ys})_j$

$(\sigma_{ys})_j$ = initial horizontal distribution of concentration from emissions in the jth subdivision

$x_{z,j}$ = "vertical" virtual distance, i.e., $\sigma_z(x_{z,j}) = (\sigma_{zs})_j$

$(\sigma_{zs})_j$ = initial vertical distribution of concentration from emissions in the jth subdivision.

This approach has an advantage over the first approach in that larger subdivisions of the area source may be used to approximate the integral. Examples of the use of this approach include Croke and Roberts (1971) and Milford, et al. (1970). If the source emissions are known in detail, the parameters σ_{ys} and σ_{zs} may be estimated by standard statistical techniques. Where detailed information is not available, it is necessary to judiciously approximate the parameters.

In the third approach, following a development proposed by Calder (1969), the assumption is made that spatial distances between variations in the area-source emission rate are large compared to the horizontal diffusion parameter σ_y. The quantity $q(x,y,h_i)$ is constant over the range of y for which the integrand in Equation 29 is significantly greater than zero. The integration limits with respect to y may be extended to infinity since $q(x,y,h_i)$ is zero outside the area source. Let

$$q'(x,h_i) = \int_{-\infty}^{\infty} \frac{q(x,y,h_i)}{\sqrt{2\pi}\,\sigma_y(x)} \exp\left\{-\frac{y^2}{2\sigma_y^2(x)}\right\} dy \qquad (36)$$

Equation 29 may be written as follows:

$$\chi_A = \sqrt{\frac{2}{\pi}} \sum_{i=1}^{3} \int_{0}^{x_1} \frac{q'(x,h_i)}{u(h_i)\ \sigma_z(x)} \exp\left\{- \frac{h_i^{\,2}}{2\sigma_z^{\,2}(x)} - \frac{0.693\ x}{t_{50}\ u(h_i)}\right\} dx \qquad (37)$$

Under the narrow plume assumption, we approximate $q'(x,h_i)$ by $q(x,o,h_i)$. This approach represents the greatest potential saving in computational effort if it can be shown to yield results sufficiently close to the double integration of the first approach.

Detailed specifications for the computational procedures used to implement the first and third approaches are listed in Appendix D. These methods were compared using model inputs generated from 10 hours of St. Louis Data, consisting of every 6th hour during a 60-hour period from December 1 to 4, 1964. The same set of input values was used for each method. Figure 8, a comparison of the concentrations predicted at 40 points by each method for one selected hour, shows the two sets of predicted concentrations tightly clustered about the equality line. The comparisons for the other hours give similar results.

Using the narrow plume approach, the computation time required on an IBM 360/65 system to compute concentrations at 10 receptor locations for 1 hour (i.e., one steady-state period with a 30 km by 40 km area source and 51 point sources) is about 1 second or 0.1 second per receptor. Using repeated application of the trapezoid rule to evaluate the double integral, the computation time is about three times as long. A large portion of the calculations required in these two methods consists of evaluating exponential factors which are saved and used repetitively in computing the terms which must be summed in the two methods.

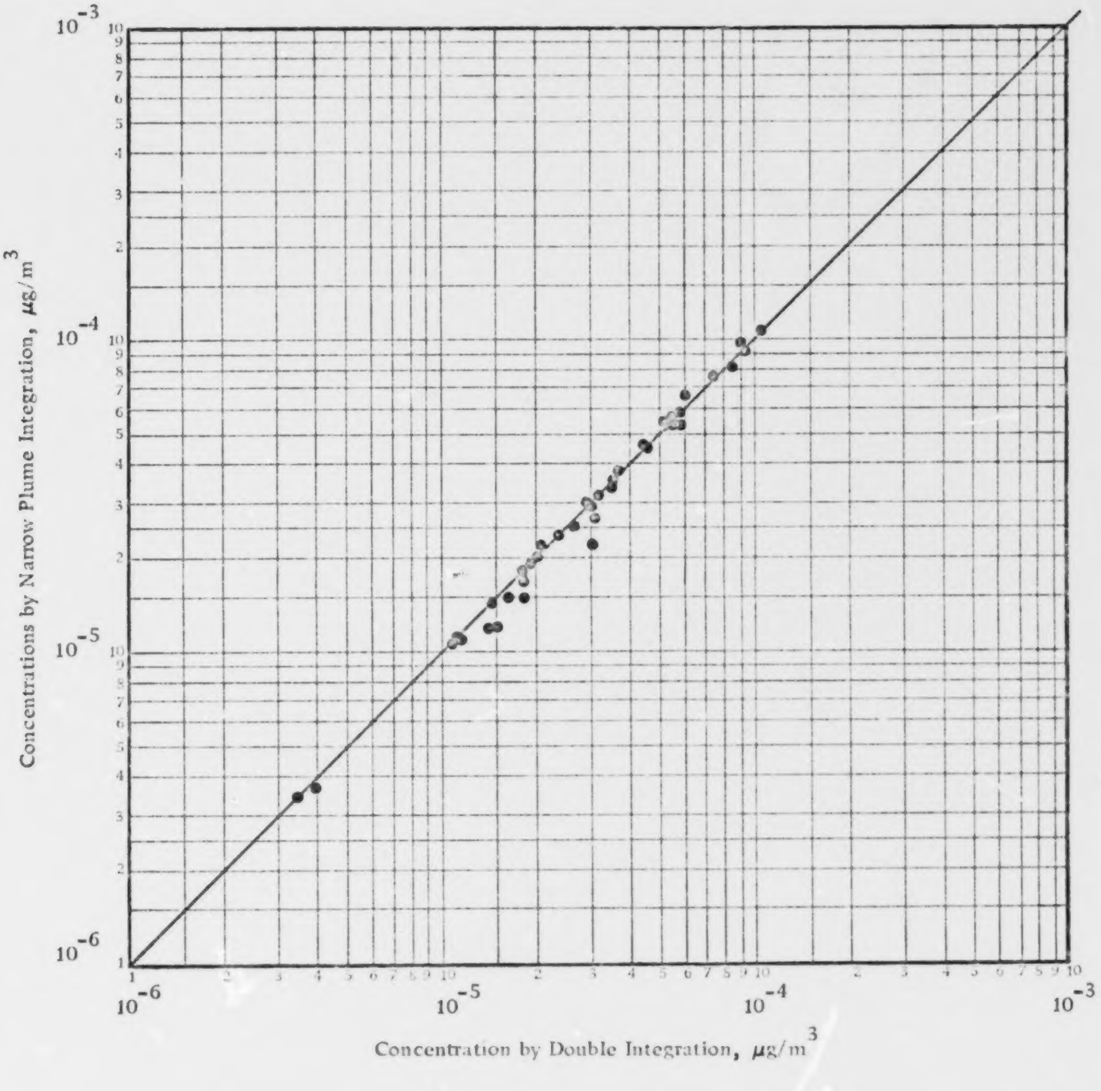


Figure 8. Comparison of Model Calculations Using Narrow Plume and Double Integration Approaches Using Portion of St. Louis Data (See Text)

The time for computing the exponential factors is about doubled in the first approach compared to the third approach. The first approach requires about six times more time to perform the remaining computations involving multiplication and summation, and approximately a 67 percent reduction in computation costs is achieved by using the third approach.

As a result of the adequacy comparisons described above between the first and third approaches, and the demonstrated economy in computer time, all computations of validity and sensitivity described in subsequent sections were conducted using the third approach, involving the "narrow plume" assumption.

3.2 COMPUTER MODEL

Having defined the mathematical structure of the diffusion model and having determined how to efficiently handle the numerical integration for area sources, it is appropriate to describe the formal organization of inputs, outputs, and data processing which has been adopted for the computer program. The relationship of the diffusion model calculations to the general data processing requirements of this study is illustrated in Figure 9. This diagram shows that there are two basic analytic frameworks in which the model is to be used: one is concerned with validation, and the other with sensitivity.

The model inputs which are required for each steady-state period are shown in Table 7. These input values may be determined by

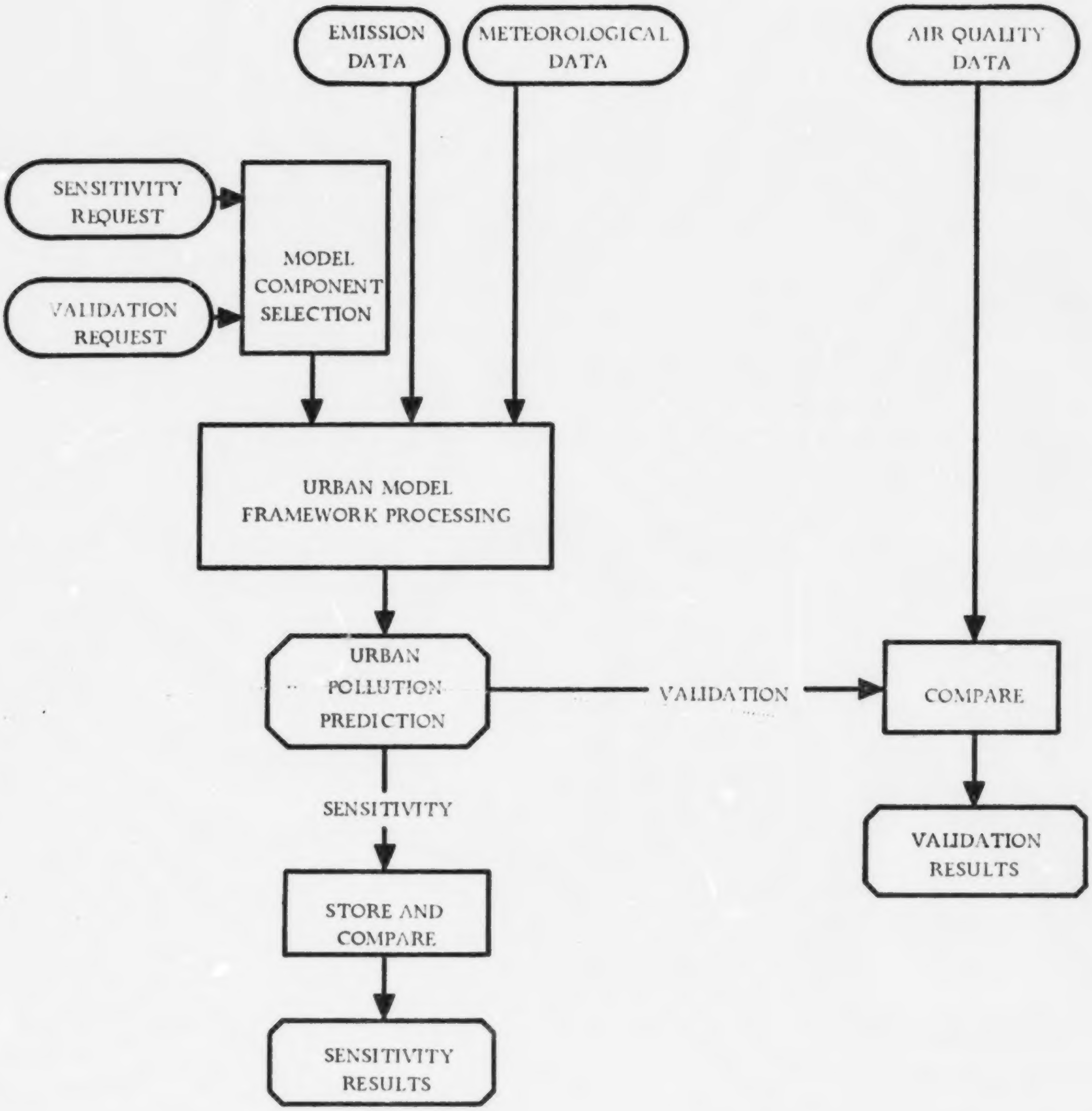

EMISSION DATA
METEOROLOGICAL DATA
AIR QUALITY DATA
SENSITIVITY REQUEST
MODEL COMPONENT SELECTION
VALIDATION REQUEST
URBAN MODEL FRAMEWORK PROCESSING
URBAN POLLUTION PREDICTION
VALIDATION
COMPARE
SENSITIVITY
VALIDATION RESULTS
STORE AND COMPARE
SENSITIVITY RESULTS

Figure 9. Data Processing for Validation and Sensitivity Analysis

Table 7. Model Inputs Required for Each Steady-State Period

Model Inputs	Symbol
A. Output Request	
1. Number of Receptor Locations	N_r
2. Receptor Coordinates	
a. North-South	ξ_j; $j = 1, \ldots N_r$
b. East-West	η_j; $j = 1, \ldots N_r$
B. Diffusion Parameter Option	I
C. Area Source Emission Data	
1. Rectangular Grid Dimensions	
a. Number of North-South Grid Squares	I
b. Number of East-West Grid Squares	J
c. Number of Emission Heights	K
d. Horizontal Grid Square Dimension	Δ
e. Emission Heights	h_k, $K = 1, \ldots K$
2. Emission Rates	q_{ijk}; $i = 1, \ldots I$; $j = 1, \ldots J$; $k = 1, \ldots K$
D. Point Source Emission Data	
1. Number of Point Sources	N_p
2. North-South Coordinate	ξ_i; $i = 1, \ldots N_p$
3. East-West Coordinate	η_i; $i = 1, \ldots N_p$
4. Effective Height	h_i; $i = 1, \ldots N_p$
5. Emission Rate	Q_i; $i = 1, \ldots N_p$
E. Meteorological Data	
1. Wind Speed Profile	
a. Reference Height	z_1
b. Reference Speed	u_1
c. Power Exponent	p
2. Wind Direction	θ
3. Stability Index	S
4. Mixing Ceiling	L
F. Pollutant Decay Half-Life	t_{50}

a number of computationally trivial preprocessing calculations which enable one to derive a set of values representative of a one-hour steady-state period. The preprocessing procedures which were selected for the validation analysis are discussed in the next section. The objective was to develop a procedure for defining model inputs which are as representative as possible of hour-to-hour variations in the characteristics of the urban environment. In all cases of input definition, determination of the best procedure to be used was made as objectively as possible on physical grounds, without regard to whether the determination would improve or worsen the validation results. It is emphasized that in no case was any empirical fitting, adjustment, or "calibration" employed. Any application of the model requires that a preprocessing program be used to convert the type and forms of available data to the inputs required by the model.

Table 7 shows that the output request consists of the number of locations for which concentrations are to be computed and their coordinates. The diffusion parameter option indicates which of three sets of diffusion parameter functions, which specifies σ_y and σ_z as a function of distance from the source, will be used. The options include the three sets discussed in Section 2.4.4, namely, the Pasquill parameters, the McElroy-Pooler parameters based on bulk Richardson number and σ_θ, and the McElroy-Pooler parameters based on the Turner stability criteria.

The area source emission data which are input to the model include the three emission rate array dimensions (I, J and K), the grid square dimension, the effective source heights, and the array of emission rates. The point source emission data include the number of point sources and, for each source, its coordinates, its effective height (the sum of its physical height and the plume rise), and its emission rate.

The meteorological data input to the model include the wind speed profile parameters (reference wind speed, reference height and power law exponent), the wind direction, the stability index value which determines which power functions to use in the selected system of diffusion parameters, and the mixing ceiling height.

The final input is the pollutant half-life (t_{50}) due to atmospheric removal processes.

Listings of the computer programs (one for numerical integration of the double integral and one for the narrow plume approach) are given in Appendix D. It should be noted that these programs are not operational entities which can be efficiently utilized outside the scope of this study, because these programs have been designed to interface with specific input and output requirements for this study. However, the programs are highly modular in structure and contain many FORTRAN coded subroutines directly applicable to any use of the Gaussian plume type of urban diffusion model. These subroutines can be evolved into more operational programs. New programs could be specifically designed from an input-output point of view to support air quality management requirements such as evaluation of implementation plans, support of land use studies, and direct aid in deciding when to implement control measures.

Section 4.0

VALIDATION ANALYSIS

The objective of the validation study was to evaluate critically the predictive accuracy of the urban diffusion model based on the Gaussian plume concept. The results tend to emphasize the general capabilities and limitations inherent in the use of the basic steady-state plume equation to simulate urban SO_2 concentrations in detail. The validation study has been based on a comparison between model predictions and urban air quality measurements of the stable pollutant SO_2. Validation data were obtained from two urban areas (St. Louis and Chicago) for which reasonably detailed emission inventory and meteorological observations were available. These two sites were selected because the available data were known to be reasonably free of errors and well organized. The St. Louis data included a three-month data collection which was part of the U.S. Public Health Service's air quality study in that area. The Chicago data consisted of a one-month set of data collected by Argonne National Laboratory. Additional Chicago data for a one-year period were reviewed but not used because of irregularities in the data and large blocks of missing data. These data collections include sufficient air quality sampling locations (10 in St. Louis and 8 in Chicago) and the most detailed source inventory information known to be available (sources summarized by square mile areas with the 50 or so largest sources identified in greater detail).

The validation analysis involves study of both short-term concentrations for 1 or 2 hours and long-term concentrations for 1 month and 3 months; these have been evaluated separately for each location (Sections 4.2 and 4.3). The analysis was carried out for individual observing stations, eight in Chicago, and 10 in St. Louis, for which short-term (1 or 2 hour) average concentrations were observed. Standard statistics have been generated regarding predicted and observed values including mean error, standard deviations (or root-mean-square errors), and empirical frequency distribution of errors for each observing station. The same statistics have been generated for the combined set of all values for a given city. Statistics have also been generated to compare predicted and observed long-term mean concentrations. The evaluation is based on the ability of the model to predict values from observed best estimates of the model inputs.

The validation is based on the use of the "narrow plume" assumption to compute concentrations from area sources (Equation 37) and the McElroy-Pooler diffusion parameters based on Turner's definitions of stability categories to represent σ_y and σ_z.

4.1 VALIDATION DATA AND PREPROCESSING TREATMENT

Special data processing procedures were used in the validation study to determine hourly values of model inputs from available data for each location. Conceptually, the processing follows the scheme illustrated by Figure 10. The raw data file consists of meteorological data, air quality data, and emission data. The meteorological data and air quality data are time-oriented. Information is available for each hour of the validation period. The emission data are source-oriented. Information is available for each point source and each square mile

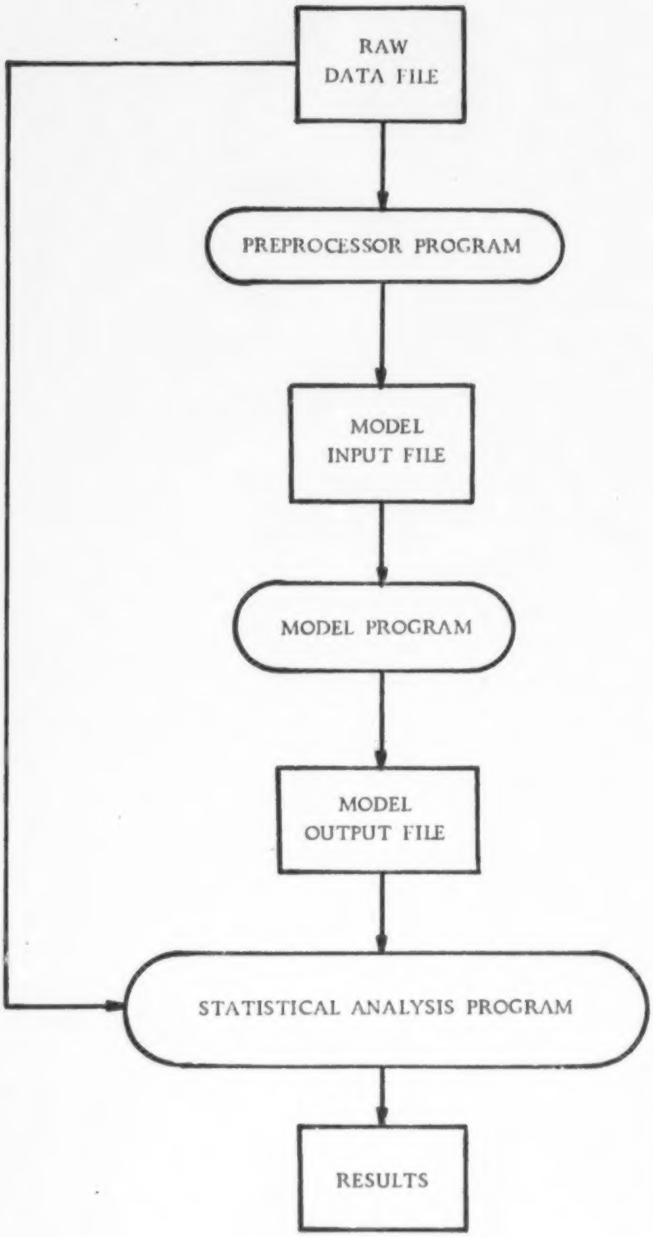

RAW
DATA FILE
PREPROCESSOR PROGRAM
MODEL
INPUT FILE
MODEL PROGRAM
MODEL
OUTPUT FILE
STATISTICAL ANALYSIS PROGRAM
RESULTS

Figure 10. Data Processing and Storage Plan for Validation Analysis

of the city area. The emission data is used in conjunction with meteorological data and time considerations (e.g., hour of the day, day of the week, and month of the year) to estimate hourly emission rates. The preprocessing program consists of a set of algorithms for deriving hourly model input values from the raw data files. The logic of the model program as it operates in the context of the validation analysis is illustrated in Figure 11. The output file created by the model program is analyzed by statistical routines to obtain the validation results.

The model inputs required for each steady-state period are listed in Table 7 in Section 3.2. The algorithms are discussed briefly below. A complete description of the emission, meteorological, and air quality data and the algorithms used to compute emission rates is given in Appendices B and C for St. Louis and Chicago, respectively. The objective has been to develop a procedure for defining model inputs which are as representative as possible of hour-to-hour variations in the characteristics of the urban environment. In all cases of input definition, determination of the best procedure to be used was made as objectively as possible on physical grounds, without regard to whether the determination would improve or worsen the validation results; in no case was any empirical fitting, adjustment, or "calibration" employed. Applications of the model to new data sources may require that a new preprocessing program be developed which will convert the type and forms of available data to the inputs required by the model.

Emission rates for point sources were estimated by one or more of three procedures. For most large utility plants, emissions were estimated on the basis of engineering information which related

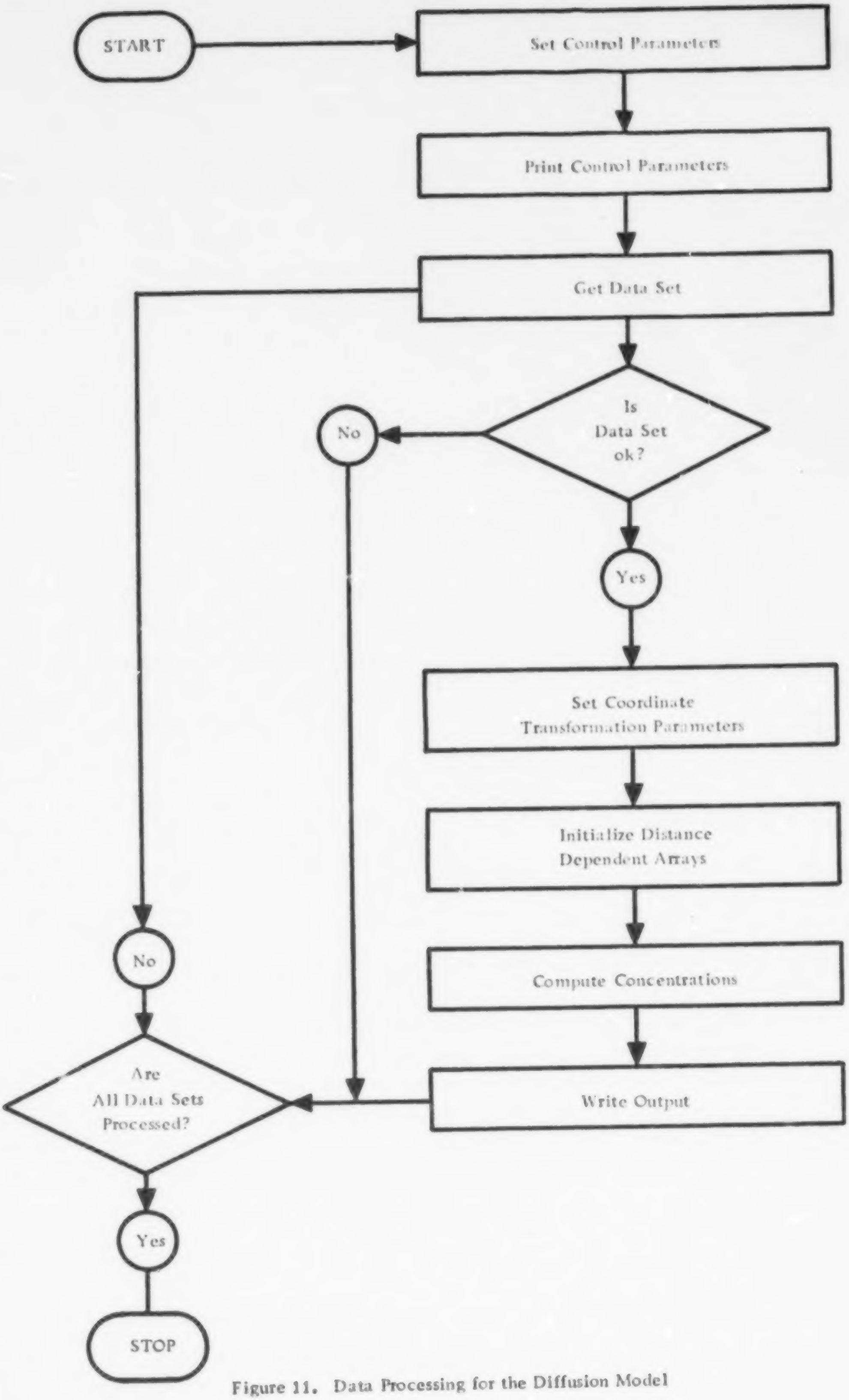

START
Set Control Parameters
Print Control Parameters
Get Data Set
Is Data Set ok?
No
Yes
Set Coordinate Transformation Parameters
Initialize Distance Dependent Arrays
Compute Concentrations
Write Output
No
Are All Data Sets Processed?
Yes
STOP

Figure 11. Data Processing for the Diffusion Model

flue gas characteristics to generating-unit output loads. The parameters of the linear relationship between fuel consumption and generator output for St. Louis data are given in Appendix B. The parameters for the Chicago data were developed by Argonne National Laboratory (Roberts, et al., 1970) with advice from Commonwealth Edison Company and used in this study by permission of the Commonwealth Edison Company. The SO_2 emission rate for each generator is

$$Q = .02S(A_1 + A_2L) \tag{38}$$

where

Q = SO_2 emission rate
S = sulfur content of fuel
L = hourly generator output load
A_1, A_2 = parameters of the relationship between fuel consumption and power generated.

The emissions from each generator are allocated to one or more stacks as appropriate (e.g., see Appendices B and C). For industrial plants, emissions due to process requirements and space heating were estimated separately. For St. Louis, the space heating requirements were related to the outside air temperature following a procedure developed by Turner (1968a). For Chicago, it was a direct correlation with outside air temperature (see Appendix C). Process emissions were related to hourly and weekly operating hours and, for Chicago, to monthly operating requirements.

For the St. Louis data, plume rise estimates were obtained from plume rise times wind-speed products, furnished by EPA for each point source, by dividing this estimate by the wind speed at the physical stack height. The EPA estimates were originally calculated from stack data using Holland's (1953) formula, which is

$$u \cdot \Delta h = V_s d \left[1.5 + 0.00268P \left(\frac{T_s - T_a}{T_s} \right) d \right] \tag{39}$$

where

$u \cdot \Delta h$ = wind speed times plume-rise product, m^2/sec

V_s = stack gas exit velocity, m/sec

d = stack exit diameter, m

P = atmospheric pressure, mb

T_s = stack gas exit temperature, °K

T_a = ambient air temperature, °K.

The values obtained were taken as representative of the entire three-month period. For the Chicago data, plume rise estimates were obtained using Briggs' formulas (1969)(see Section 2.3.2 of this report). Heat emission estimates were obtained by assuming that 15 percent of the heat content of consumed fuel is contained in the flue gases.

Area source emissions are represented by a three-dimensional matrix of emission rates. The dimensions of the matrix correspond to three effective source heights and the two dimensions of a horizontal grid work of square mile blocks. The available emission inventory data for each square mile include emissions associated with space heating which are taken to be proportional to the temperature deficit from 65°F in accordance with Turner's (1968a) technique, and emissions (for St. Louis) associated with commercial and industrial sources which are time-of-day oriented. The specific algorithms used to make hourly area source emission rate estimates are given in Appendices B and C for St. Louis and Chicago, respectively.

The model requires a single steady-state wind direction and wind speed profile for each one-hour period. A vector mean average of the observations from several locations was used as the mean wind direction and speed. For St. Louis, wind observations at three levels on a 425-foot tower were used to empirically determine the wind profile power law. When vertical profiles were not observed, a power law of 0.1, 0.15, 0.2, 0.25 or 0.3 was assigned corresponding to the calculated diffusion stability class (A to E, as defined in Tables 2 and 3). Since vertical wind profiles were not available for the Chicago analyses, the profile power law was estimated from the stability class. A value of 0.1 was assigned for classes A and B, 0.15 for class C, 0.2 for class D and 0.3 for class E. The change from the St. Louis values was used to account for the increased surface roughness around the Chicago area. Although the validation study is based on the use of wind speeds and directions determined as the vector average of several observations, there is close agreement between these winds and the nearest airport winds. It is assumed that the validation findings would not be significantly changed by the use of a single airport wind observation. However, for light wind situations with wind speeds less than 5 mph, differences are more frequent. The validity of the model using a single airport wind might be decreased from the results shown in this study at locations where light winds occur frequently.

The mixing layer ceiling was estimated by interpolating between mixing layer heights indicated by radiosonde observations made within 100 to 200 miles of each city. For St. Louis, the mixing layer height was the average of daily estimates furnished by Environmental Protection Agency for Columbia, Missouri, and Peoria, Illinois. Values for times between the early morning minimum and the afternoon maximum (see Figure 7) were obtained by linear interpolation. The afternoon maximum was retained until midnight, after which the early morning value of the following day was assumed. For Chicago, hourly estimates were obtained from Argonne. These ceilings were constructed (Roberts, et al., 1970) by interpolating between the Green Bay, Wisconsin and Peoria, Illinois morning and afternoon radiosondes to define hourly vertical temperature profiles. The mixing ceiling for each hour is defined by the height of the intersection of a dry adiabatic projection from the urban surface temperature with the interpolated temperature profile.

An urban diffusion stability index was computed using airport weather observations according to the rules outlined by Turner (1964) (see Tables 2 and 3 of this report). For St. Louis the airport weather observations were taken at Lambert Field. For Chicago the airport weather observations were taken at Midway Airport.

4.2 RESULTS OF SHORT-TERM (ONE- AND TWO-HOUR) VALIDATION CALCULATIONS

Validation results were calculated with the "narrow plume" version of the multiple-source steady-state Gaussian plume model using hourly values of all parameters, including emission rates. In this model, the largest sources are treated as point sources. All other sources are treated as an area source with emissions at one or more of three effective source heights. The method of calculation is described in Section 3.1 and Appendix D. The initial data and preprocessing treatment used to produce model inputs are described in Section 4.1 and Appendices B and C.

4.2.1 Comparisons with St. Louis Data

The St. Louis comparisons cover the three months from 1400 December 1, 1964, to 1400 February 28, 1965. The sampling operation by which the observed St. Louis values were obtained was described by Turner and Edmisten (1968). Hourly calculations were made for 10 sampler locations (shown in Figure 12). The location of the airport weather observing station (Lambert Field), the TV tower for vertical wind profile observations, and the three continuous wind measuring stations are also shown in Figure 12.

Figures 13 through 16 are selected examples showing model performance on a two-hour basis. At each station two, one-hour predictions are averaged and compared with the corresponding two-hour SO_2 observations:

- Figure 13 is a typical example of combined over- and underprediction which may be found side-by-side during a single two-hour period. The upper number is the observed value and the lower number is the predicted value.

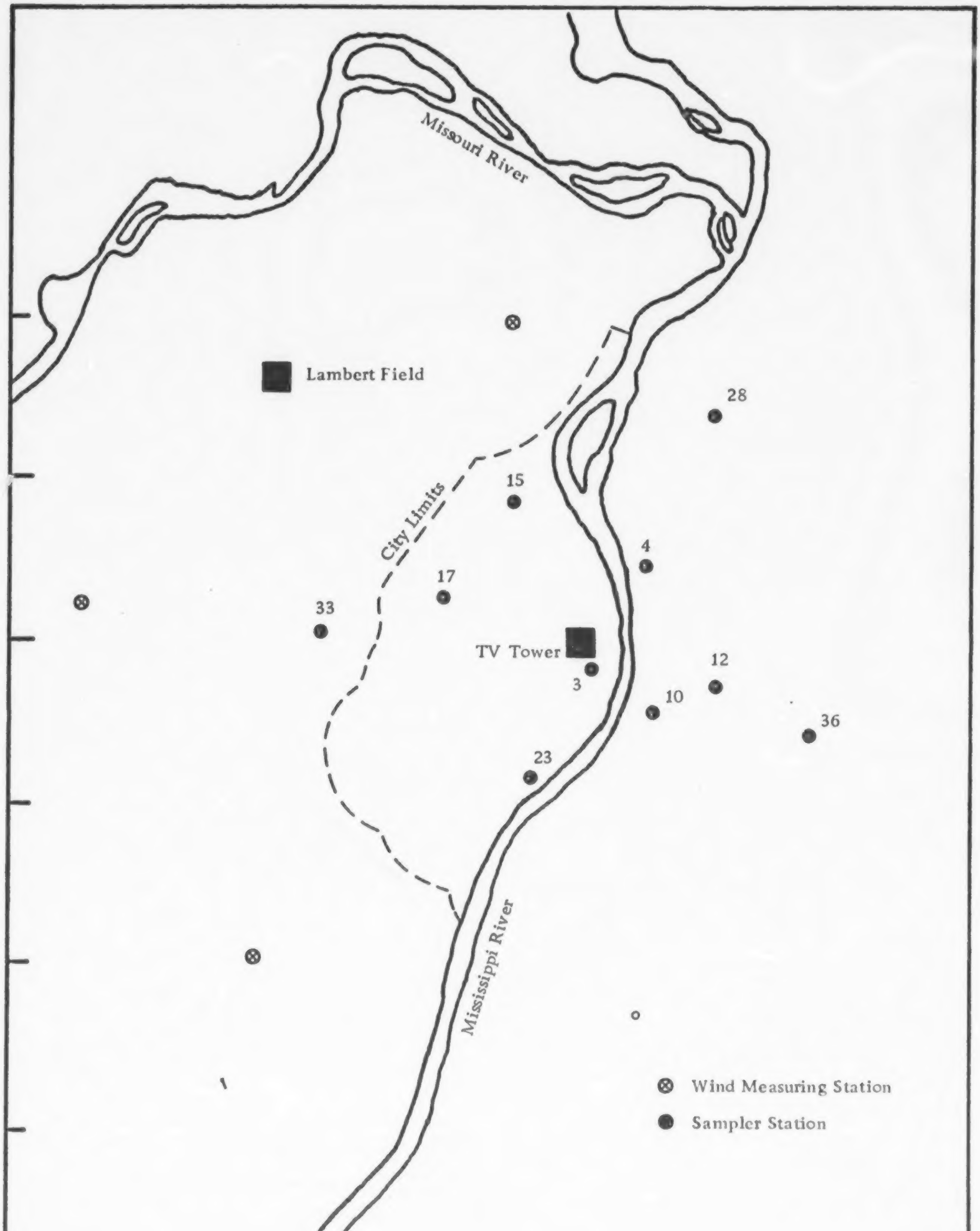

Missouri River
Lambert Field
28
15
City Limits
4
17
33
TV Tower
3
12
10
36
23
Mississippi River
⊗ Wind Measuring Station
● Sampler Station

Figure 12. Location of St. Louis Observing Stations Used in Validation Analysis

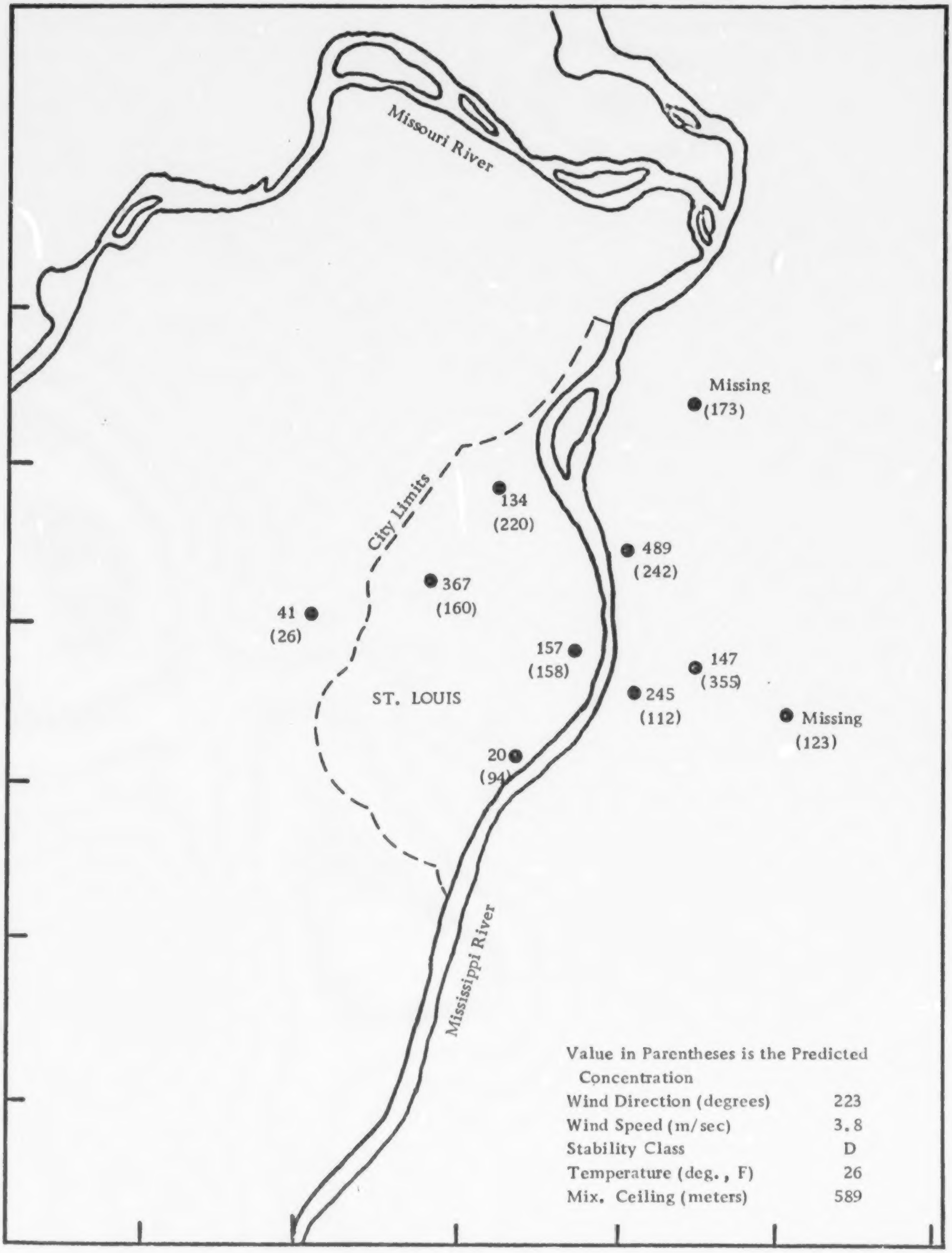

Missouri River
Mississippi River
City Limits
ST. LOUIS
Missing
(173)
134
(220)
489
(242)
367
(160)
41
(26)
157
(158)
147
(355)
245
(112)
Missing
(123)
20
(94)
Value in Parentheses is the Predicted Concentration
Wind Direction (degrees) 223
Wind Speed (m/sec) 3.8
Stability Class D
Temperature (deg., F) 26
Mix. Ceiling (meters) 589

Figure 13. Typical Example of Predicted and Observed Concentrations in the Vicinity of St. Louis for a Two-Hour Period (Average of 7 a.m. and 8 a.m., December 7, 1964)

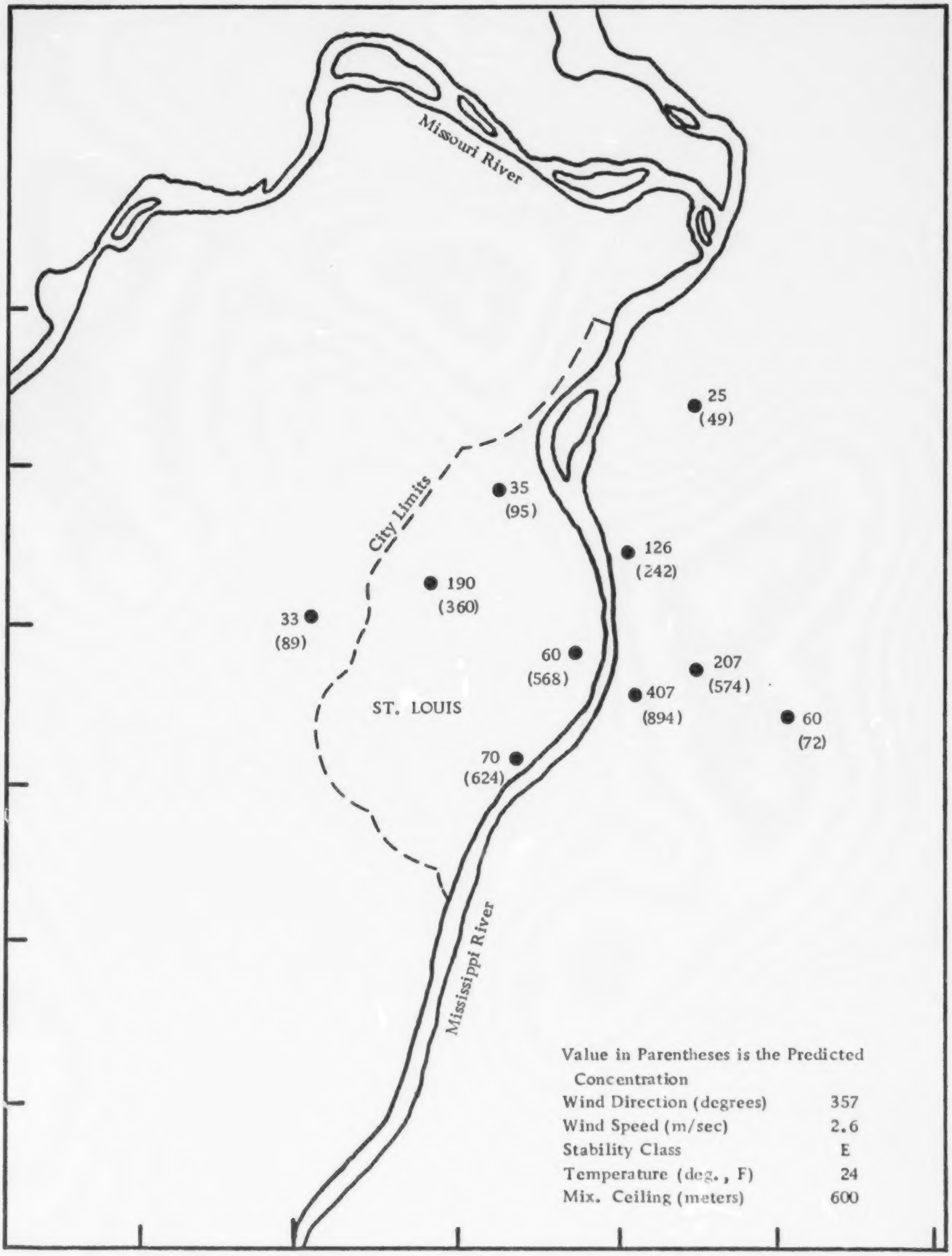
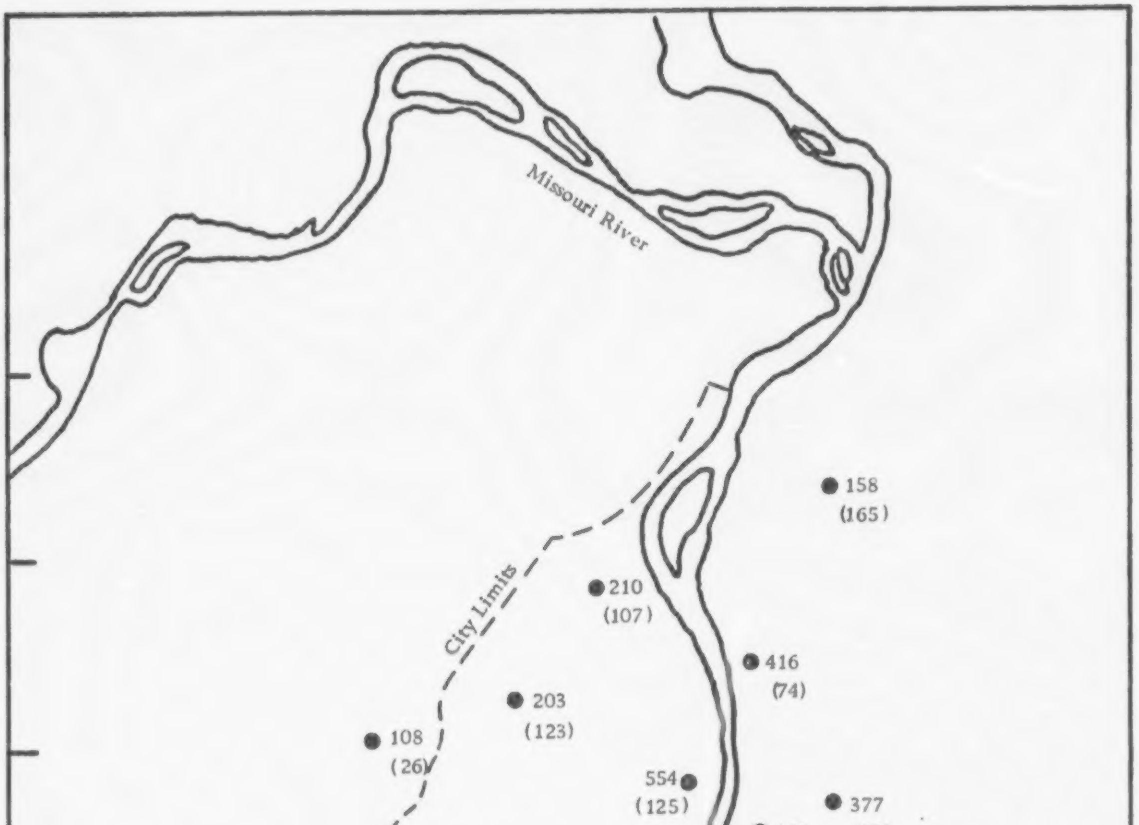

Missouri River
City Limits
ST. LOUIS
Mississippi River
25 (49)
35 (95)
126 (242)
190 (360)
33 (89)
60 (568)
207 (574)
407 (894)
60 (72)
70 (624)
Value in Parentheses is the Predicted Concentration
Wind Direction (degrees) 357
Wind Speed (m/sec) 2.6
Stability Class E
Temperature (deg., F) 24
Mix. Ceiling (meters) 600

Figure 14. Example of Overpredictions in the Vicinity of St. Louis During a Two-Hour Period of Stable Conditions (Average of 1 a.m. and 2 a.m., December 15, 1964)


Missouri River
City Limits
ST. LOUIS
Mississippi River
158
(165)
210
(107)
416
(74)
203
(123)
108
(26)
554
(125)
377
(53)
468
(186)
73
(14)
38
(17)

Value in Parentheses is the Predicted Concentration

Wind Direction (degrees)	180
Wind Speed (m/sec)	3.7
Stability Class	D
Temperature (deg., F)	36
Mix. Ceiling (meters)	641

Figure 15. Example of Underprediction in the Vicinity of St. Louis During a Two-Hour Period with Southerly Winds (Average of 1 a.m. and 2 a.m., December 12, 1964)

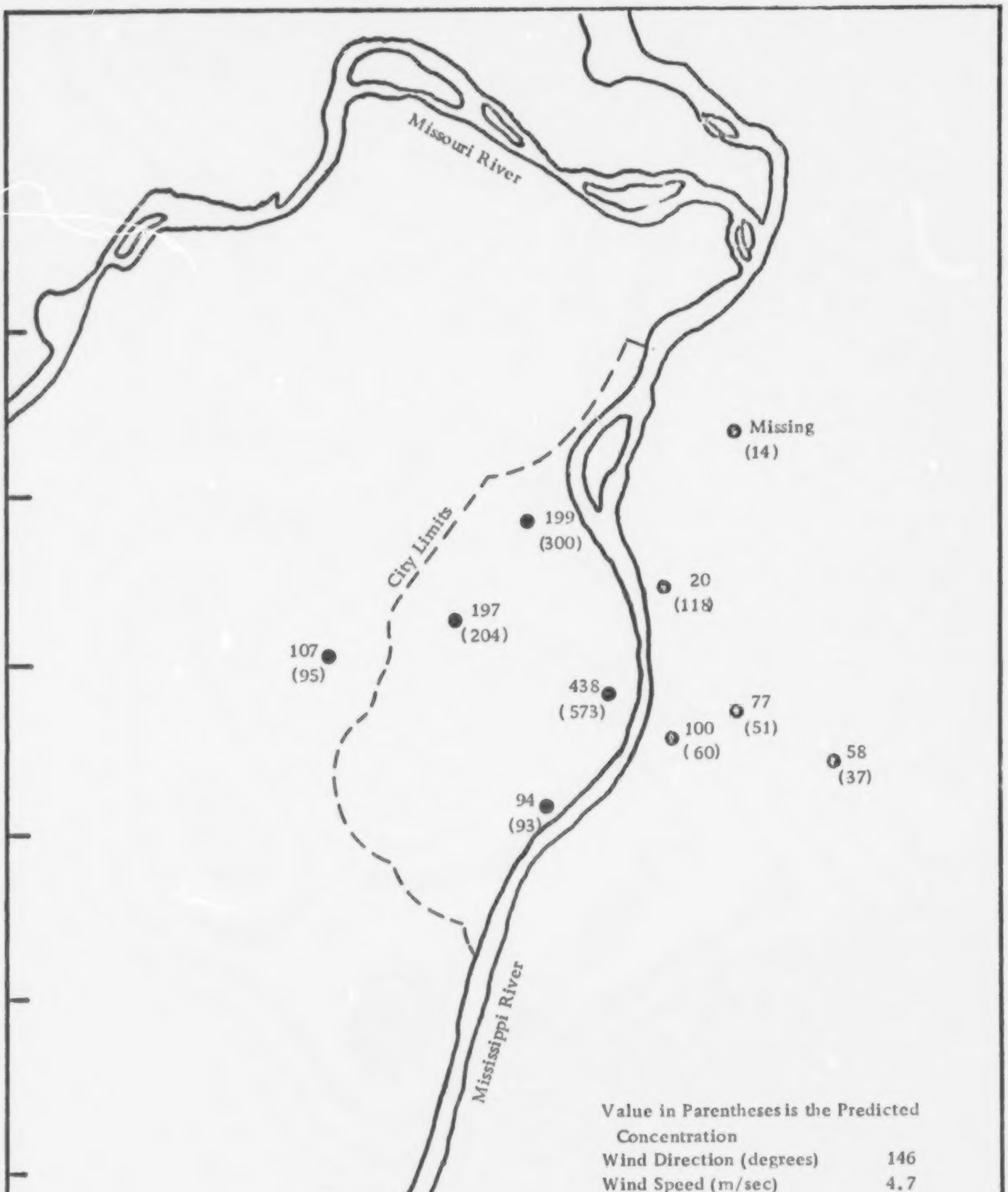

Missouri River
City Limits
Mississippi River
Missing
(14)
199
(300)
20
(118)
197
(204)
107
(95)
438
(573)
77
(51)
100
(60)
58
(37)
94
(93)
Value in Parentheses is the Predicted Concentration
Wind Direction (degrees) 146
Wind Speed (m/sec) 4.7
Stability Class D
Temperature (deg., F) 42
Mix. Ceiling (meters) 338

Figure 16. Example of Good Correspondence Between Predicted and Observed Concentrations During a Two-Hour Period (Average of 3 p.m. and 4 p.m., December 9, 1964)

- Figure 14 illustrates over-prediction. This case is an example of a Turner stability class E situation. It may be noted in passing that the model is very sensitive to changes in stability class. A change from class D to class E results in the prediction increasing by a factor of 2 to 5. This subject is treated at greater length in Section 5.4.

- Figure 15 illustrates underprediction. It was noted that underprediction generally occurred with a south wind and with unseasonably warm temperatures. There may be an error in the emission algorithms under these circumstances, in that the operation of furnaces for space heating may not follow the temperature relationship indicated by the emission algorithm. For example, furnaces in commercial and apartment buildings may be improperly adjusted for the unseasonably warm temperatures.

- Figure 16 illustrates generally good correlation between predicted and observed values at most stations.

Comparisons of two-hour concentrations were made for all ten stations for the three-month period in the St. Louis data set. A statistical summary of the validation results obtained by comparing model predictions with observations is shown in Table 8 and Figures 17 through 22 for these stations. For each station individually, and for all stations combined, a mean value and standard deviation were obtained for observed, predicted, and observed minus predicted values.

In general the mean observed and predicted values for individual stations, shown in Table 8, are in good agreement. However, this agreement is more indicative of the model's ability to predict long-term rather than short-term concentrations. The overall frequency

Table 8. Statistical Summary of Predicted and Observed Two-Hour Concentrations [(a)] for St. Louis Stations

Station Number	Mean			Standard Deviation			Mean Absolute Difference of Observed Minus Predicted	Regression of Observed on Predicted Values		Number of Values	Correlation Coefficient
	Observed Values	Predicted Values	Observed Mean Minus Predicted Mean	Observed Values	Predicted Values	Observed Minus Predicted Values		Slope	Intercept		
3	156	196	- 40	145	180	207	130	0.1637	123.9	1037	0.203
4	175	142	+ 33	157	195	212	116	0.2354	141.4	872	0.292
10	335	207	+128	237	165	255	201	0.3373	265.2	975	0.235
12	179	211	- 31	136	214	194	121	0.2891	118.4	980	0.455
15	137	118	+ 19	132	119	133	87	0.4964	78.6	900	0.448
17	211	181	+ 31	124	161	161	114	0.2973	157.7	1031	0.386
23	90	191	-101	106	241	238	142	0.1085	69.2	963	0.247
28	87	94	- 7	117	149	152	80	0.2849	60.1	788	0.363
33	73	61	+ 11	88	99	103	53	0.3517	51.1	922	0.396
36	80	88	- 8	78	134	122	64	0.2542	57.2	952	0.437
All	154	151	+ 3	159	179	194	112	0.3085	107.9	9420	0.347

(a) Units are $\mu g/m^3$.

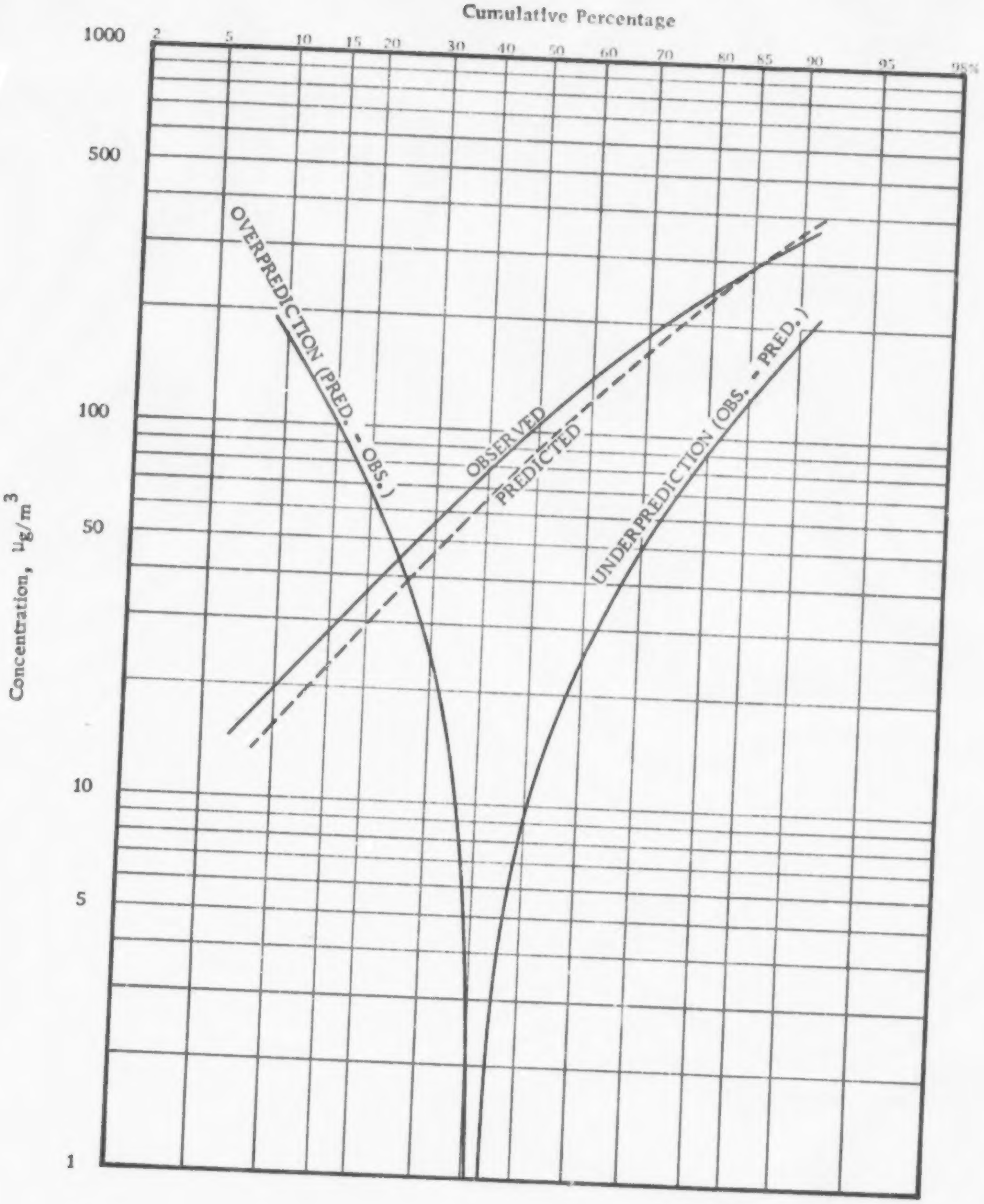


Figure 17. Frequency Distributions of Observed, Predicted and Observed-Minus-Predicted Two-Hour Concentrations for Ten St. Louis Stations Combined

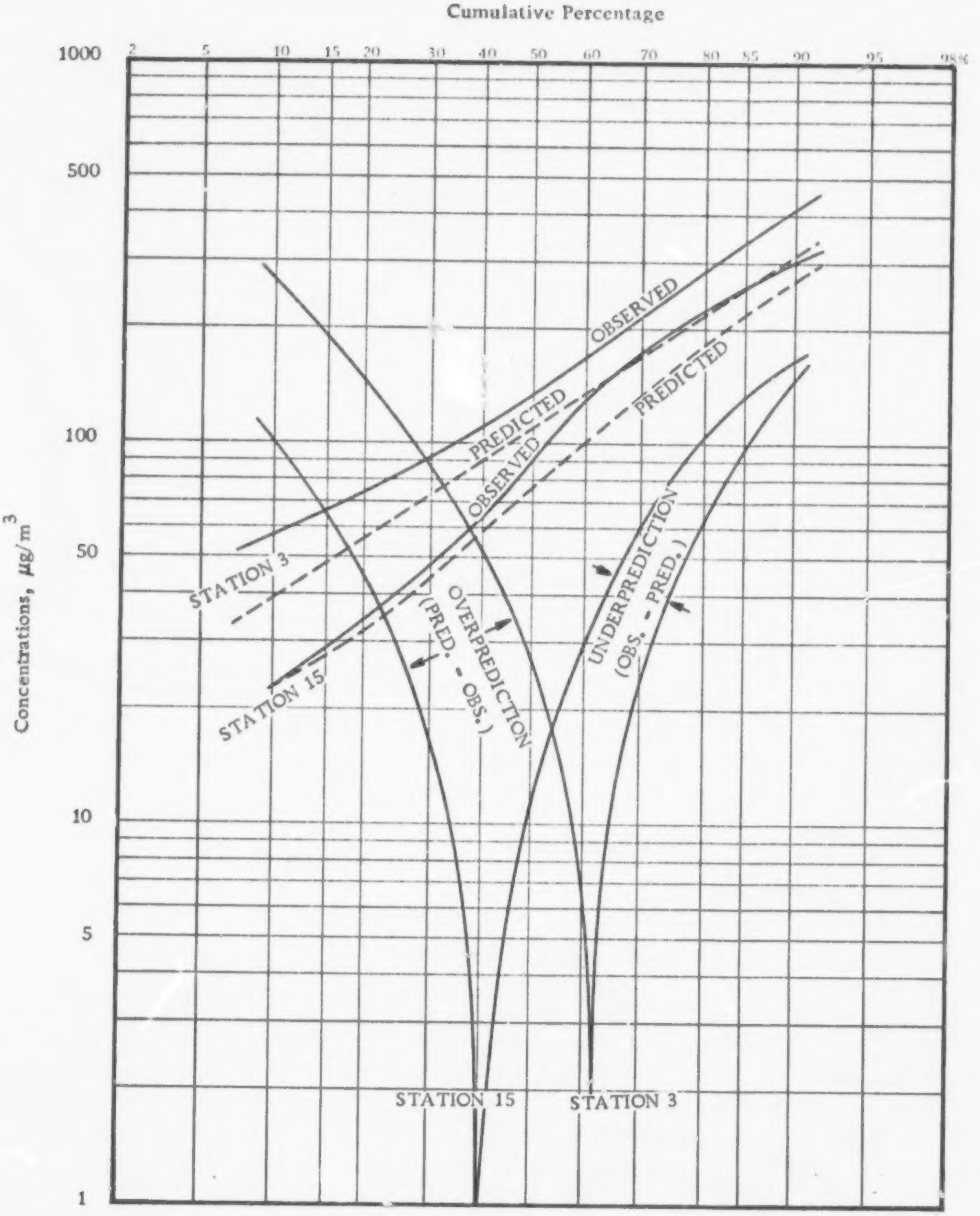


Figure 18. Frequency Distributions of Observed, Predicted and Observed-Minus-Predicted Two-Hour Concentrations for St. Louis Stations 3 and 15

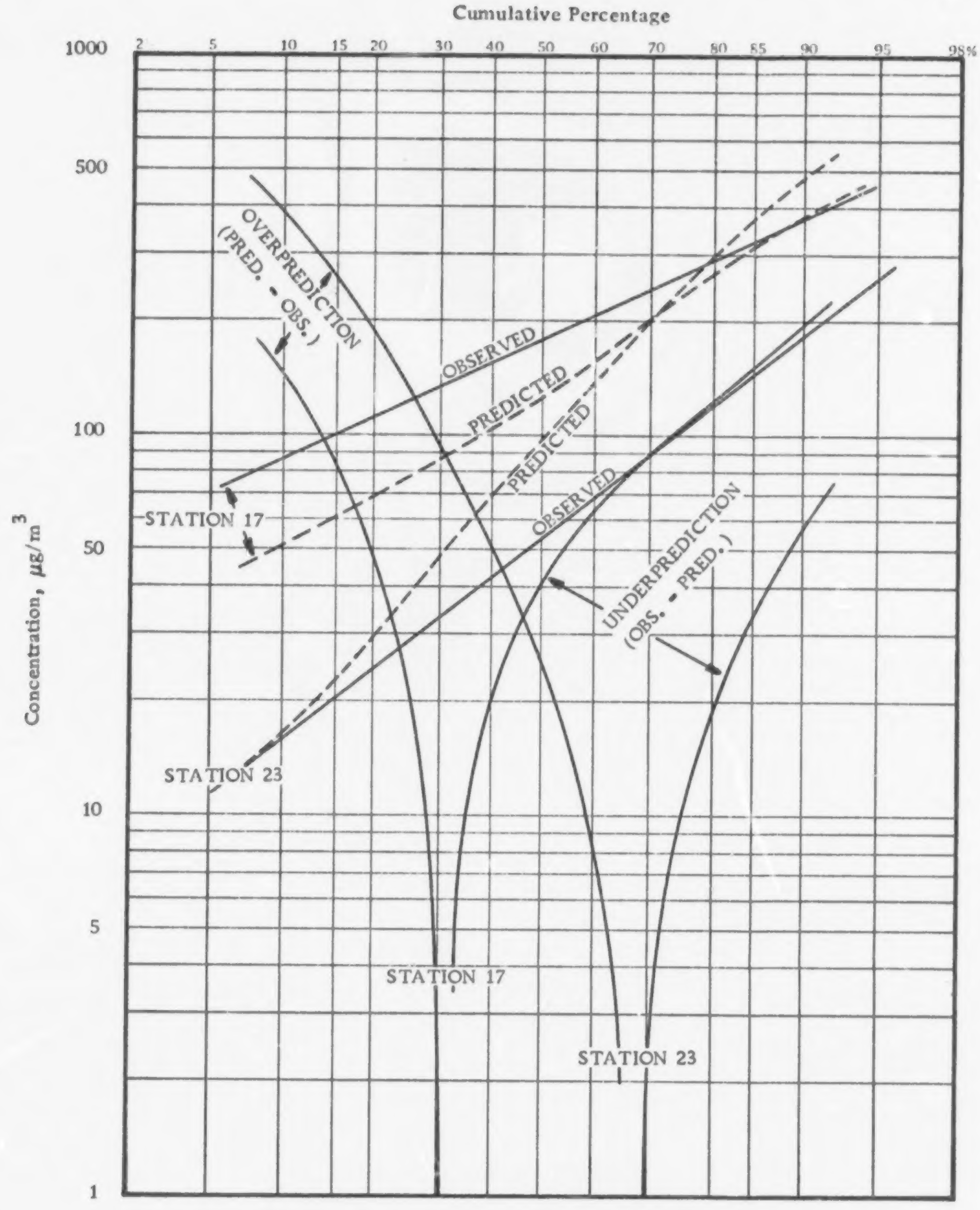


Figure 19. Frequency Distributions of Observed, Predicted and Observed-Minus-Predicted Two-Hour Concentrations for St. Louis Stations 17 and 23

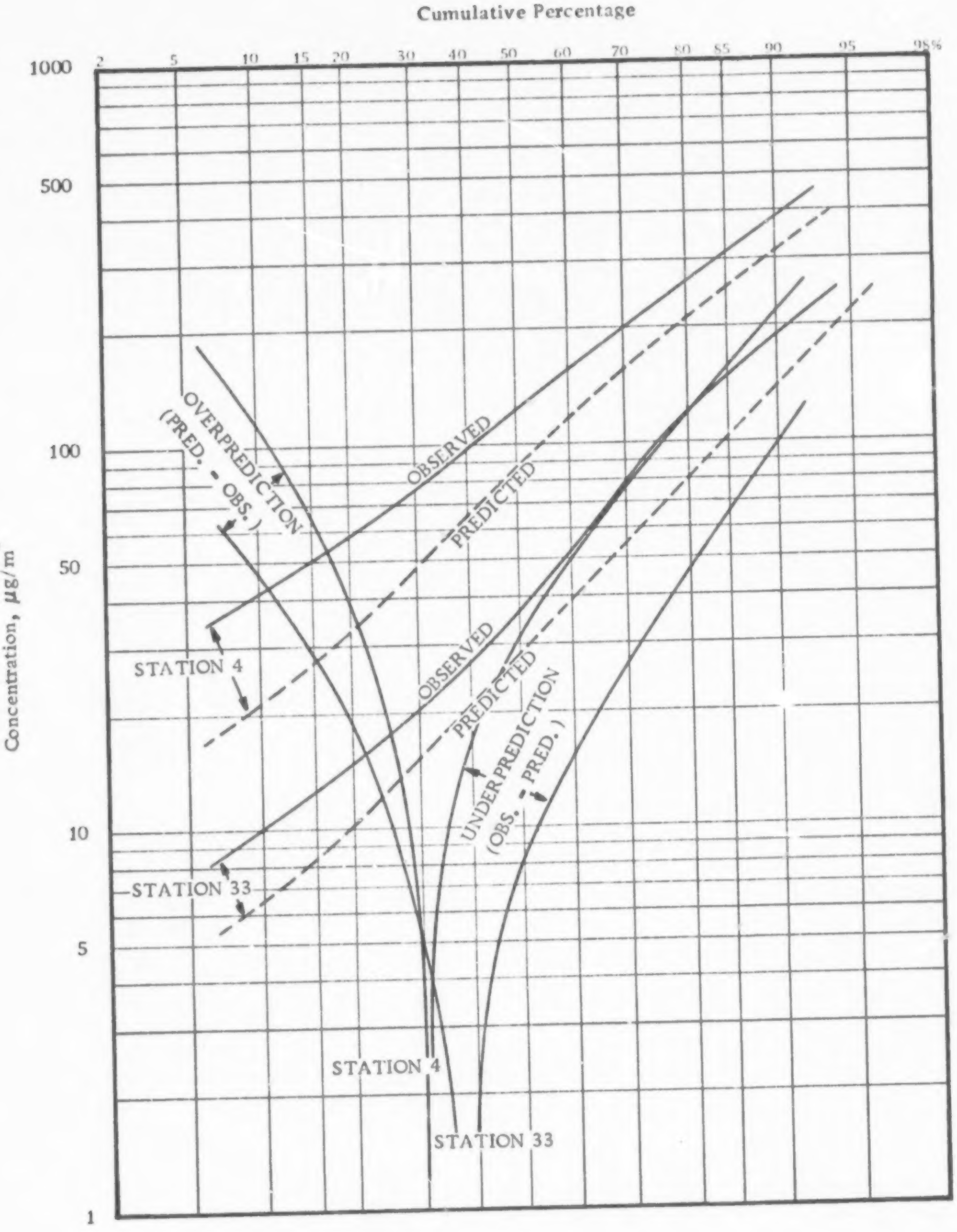


Figure 20. Frequency Distribution of Observed, Predicted, and Observed-Minus-Predicted Two-Hour Concentrations for St. Louis Stations 4 and 33

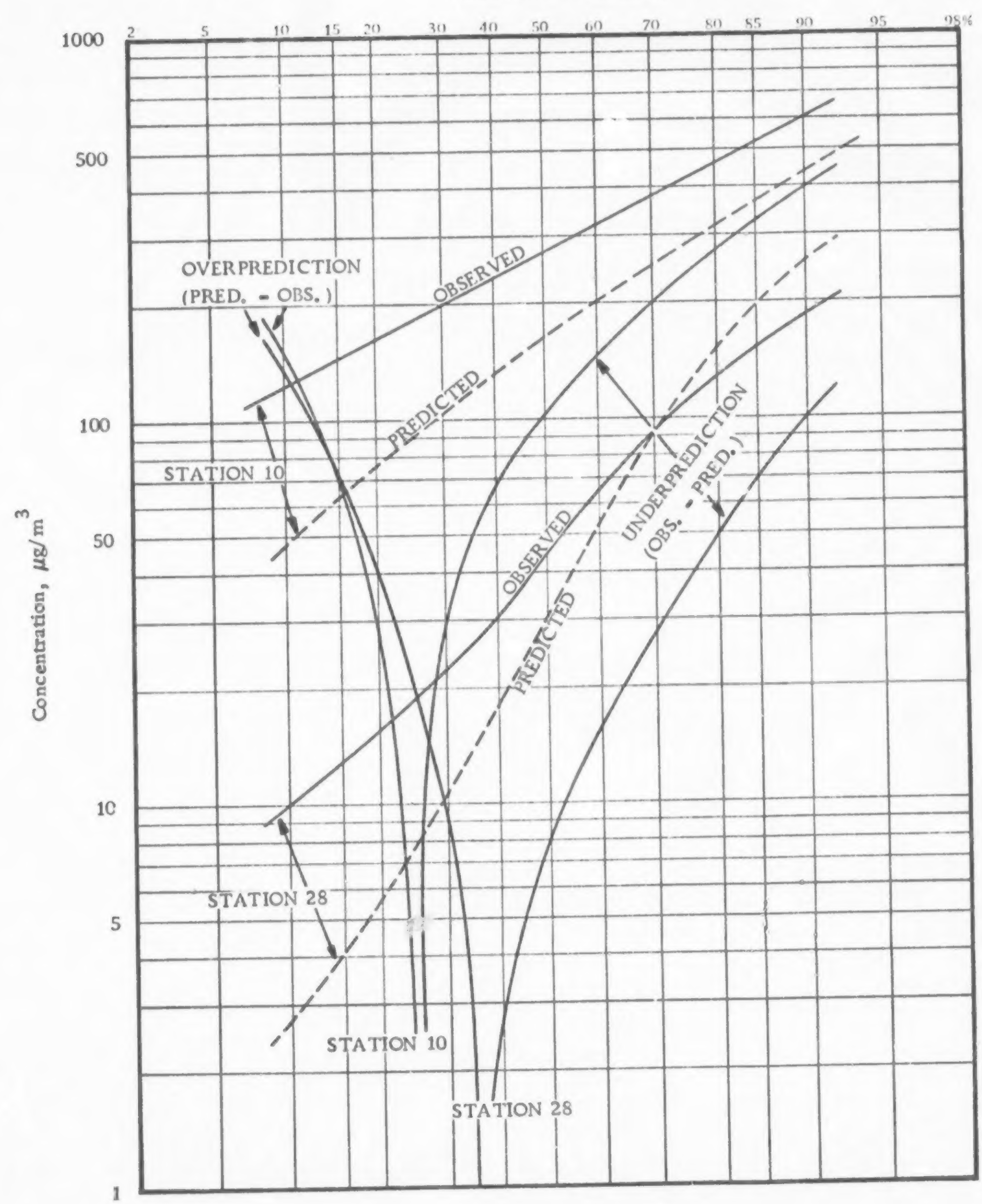


Figure 21. Frequency Distribution of Observed, Predicted and Observed-Minus-Predicted Two-Hour Concentrations for St. Louis Stations 10 and 28

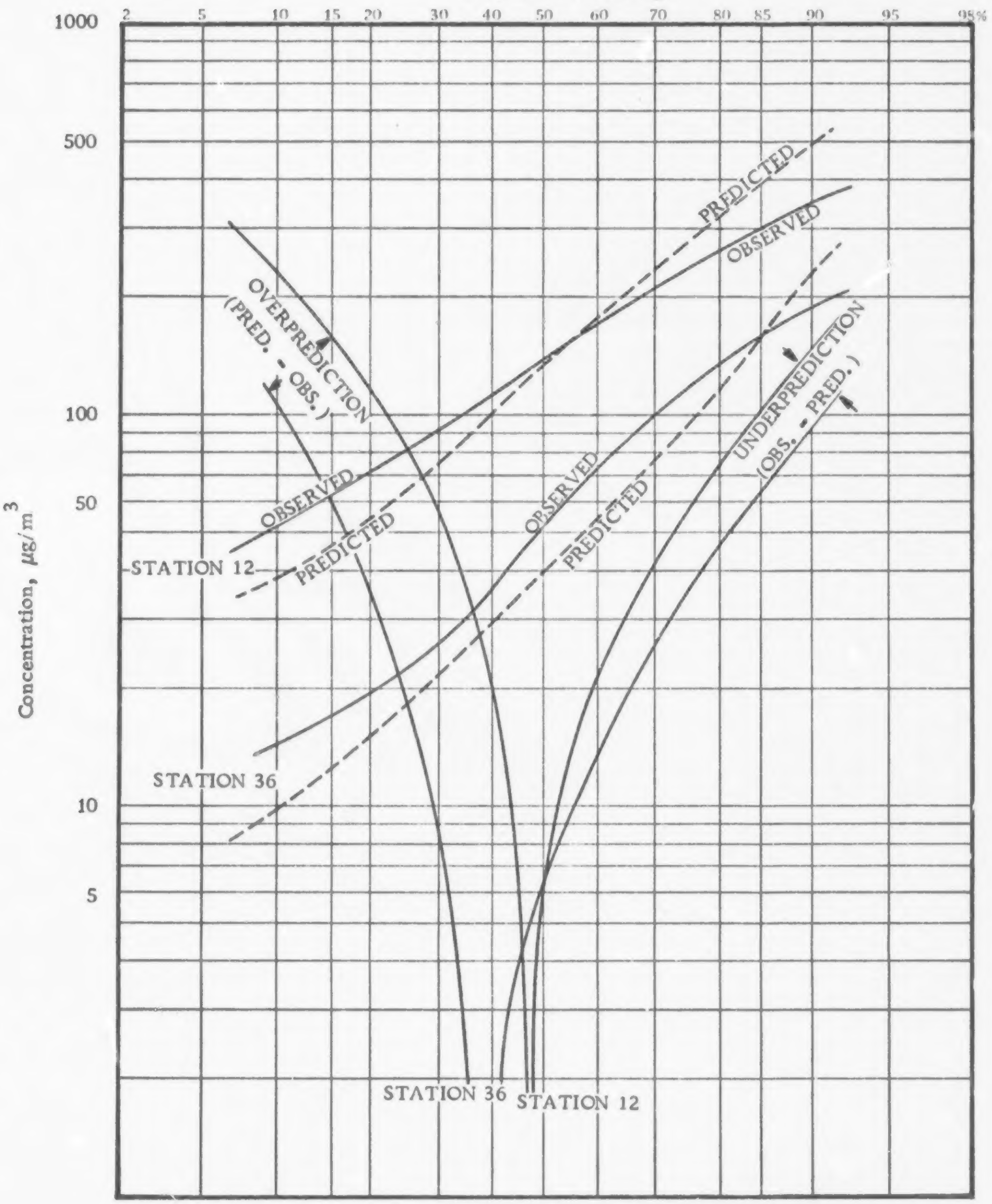


Figure 22. Frequency Distribution of Observed, Predicted, and Observed-Minus-Predicted Two-Hour Concentrations for St. Louis Stations 12 and 36

distributions of predicted two-hour concentrations for the 89-day period at individual stations is in good agreement with the overall distributions of observed two-hour concentrations. This may be seen in Figures 18 through 22. However, the agreement between predicted and observed values for any single two-hour period is not nearly as good as the overall agreement might suggest. The magnitude of individual differences is shown by the standard deviations and mean absolute differences of observed minus predicted values in Table 8. This error with regard to individual two-hour time periods is also evident in the shallow slopes and high intercept values obtained for the regression coefficients of observed on predicted values. A more detailed accounting of the error distribution of observed minus predicted values is shown for each individual station in Figures 18 through 22. These curves are labeled as "over-" and "underpredicted" in each graph. To make all differences positive for presentation on logarithmic scale, overpredictions are shown as predicted minus observed values.

The frequency distribution of the combined set of all predicted two-hour concentrations is shown in Figure 17 to correspond very closely with the observed frequency distribution. The observed and predicted means of all stations combined are 154 and 151 $\mu g/m^3$, respectively. The standard deviations are 159 and 179 $\mu g/m^3$, respectively, as shown in Table 8. In Figure 17, the fact that the curves for overpredictions and underpredictions are approximately symmetrical and meet a little below the 50 percent line (about 40-45 percent) indicates that there is no particular tendency to over- or underpredict. The figure also indicates that 50 percent of the observed values lie within ± 60 μg/m^3 of the predicted values. This is in relation to a mean predicted value of 151 μg/m^3. About 65 percent of the observed values lie within ± 100 μg/m^3 of the predicted value. The majority of the differences between predicted and observed values are noticeably smaller than the overall mean values. These predictions are not adjusted or scaled to the observed values. The individual station curves reflect the variety of results which contribute to this finding.

4.2.2 Comparisons with Chicago Data

Observed and calculated short-term (one-hour) concentrations were obtained for eight TAM (Telemetered Air Monitoring) stations in the Chicago area based on data collected for the period 0000 January 1, 1967 to 2300 January 31, 1967. These locations are shown in Figure 23.

The Chicago monitoring equipment automatically records five-minute average SO_2 concentrations. At 15-minute intervals the average concentration for the preceding 15-minute period is telemetered to a central location where it is recorded on tape. The original data tapes have been edited by Argonne National Laboratory to obtain hourly averages, by averaging five sequential 15-minute observations. The middle of the third 15-minute period of each hour was centered on the hour. A description of the Chicao TAM network was reported by Booras and Zimmer (1968). The SO_2 monitoring was done with continuous conductivity analyzers. In these instruments, air is continuously admitted to an

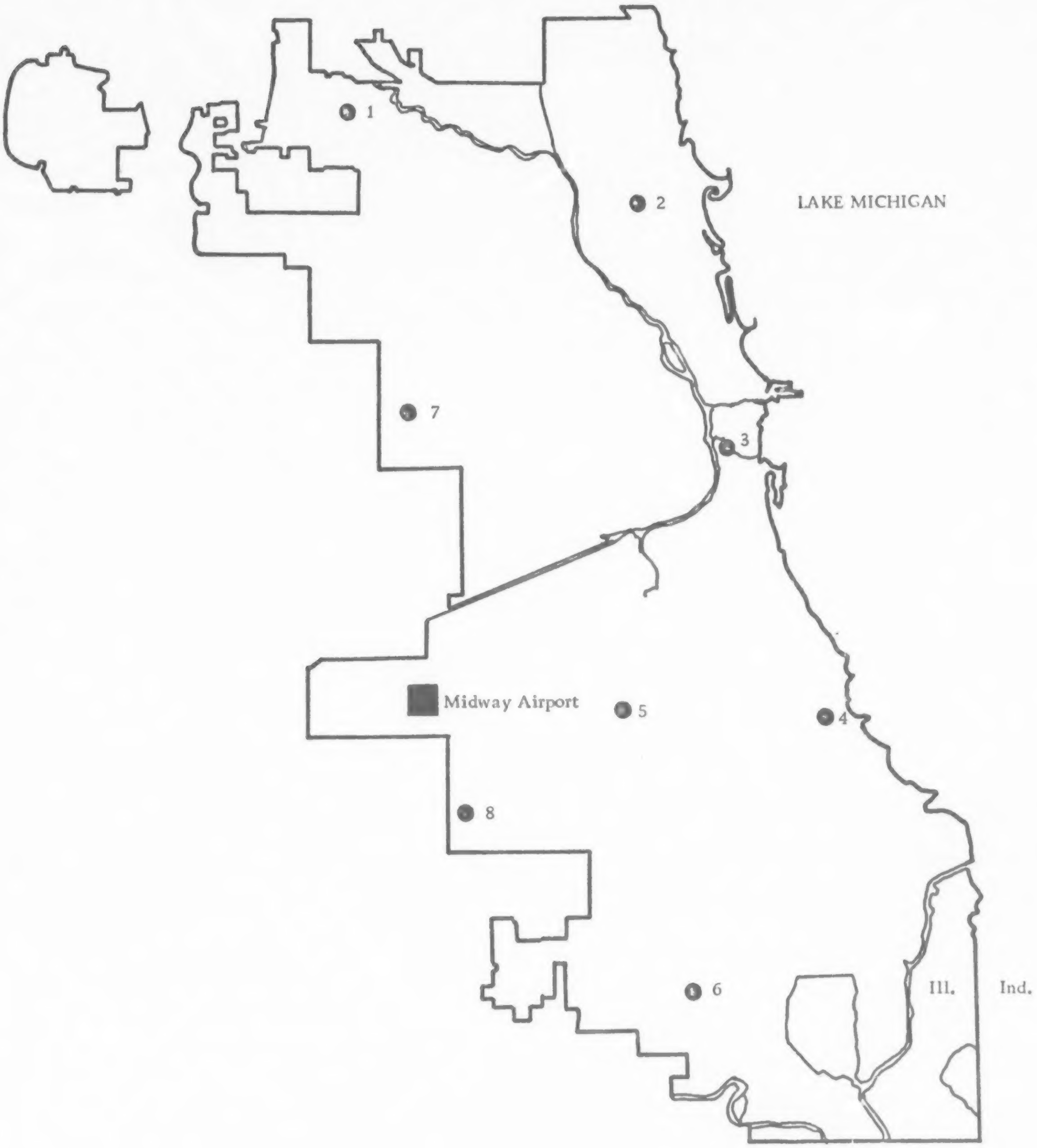

1
2
LAKE MICHIGAN
7
3
Midway Airport
5
4
8
6
Ill.
Ind.

Figure 23. Location of Chicago TAM Stations Used in Validation Analysis

absorber where SO_2 in the airstream is removed by a continuously flowing liquid absorbent. The electrical conductivity of the resulting solution is continuously measured and recorded. The readings are directly proportional to SO_2 concentrations. An integrated five-minute average is obtained automatically.

A statistical summary of the results of comparisons of the model predictions with the one-hour Chicago observations is given in Table 9, and in Figures 24-28 (similar to the St. Louis summary in Section 4.2.1).

As shown in Table 9, the predicted concentrations were on the average higher than the observed concentrations at six of the eight stations. In addition, the standard deviations of predicted values at each station were larger than the standard deviations of observed values by a factor varying between 2 and 3. The frequency distributions of observed and predicted values, and the over- and underpredictions of the observed minus predicted concentrations for individual stations are shown in Figures 25 through 28. The frequency distributions of predicted and observed values for stations 4, 5, 6, and 7 in Figures 26, 27, and 28 show that for these stations high concentrations are predicted more frequently than they are observed and low concentrations are observed more frequently than they are predicted. In Figure 28 the predominant difference between predicted and observed frequency distributions for station 8 is the high frequency of predicted low concentrations compared

Table 9. Statistical Summary of Predicted and Observed One-Hour Concentrations[a] for Chicago Stations

TAM[b] Station Number	Mean			Standard Deviation			Mean Absolute Difference of Observed Minus Predicted	Regression of Observed on Predicted Values		Number of Values	Correlation Coefficient
	of Observed Values	of Predicted Values	Observed Mean Minus Predicted Mean	of Observed Values	of Predicted Values	of Observed Minus Predicted Values		Slope	Intercept		
1	33	47	- 14	56	111	98	39	0.2349	21.6	723	0.466
2	114	99	+ 15	87	108	128	87	0.1188	102.7	602	0.148
3	312	379	- 67	152	416	397	221	0.1106	269.7	606	0.303
4	123	315	-192	89	294	274	201	0.1119	88.0	614	0.370
5	62	128	- 66	47	140	135	83	0.0936	50.2	722	0.279
6	23	58	- 35	32	98	97	45	0.0595	19.5	703	0.182
7	102	158	- 55	95	159	157	100	0.1905	72.2	711	0.319
8	43	36	+ 7	39	76	83	45	0.0366	41.8	726	0.071
All	96	145	- 49	117	232	201	99	0.2493	60.2	5407	0.494

(a) Units are $\mu g/m^3$.

(b) Telemetered Air Monitoring.

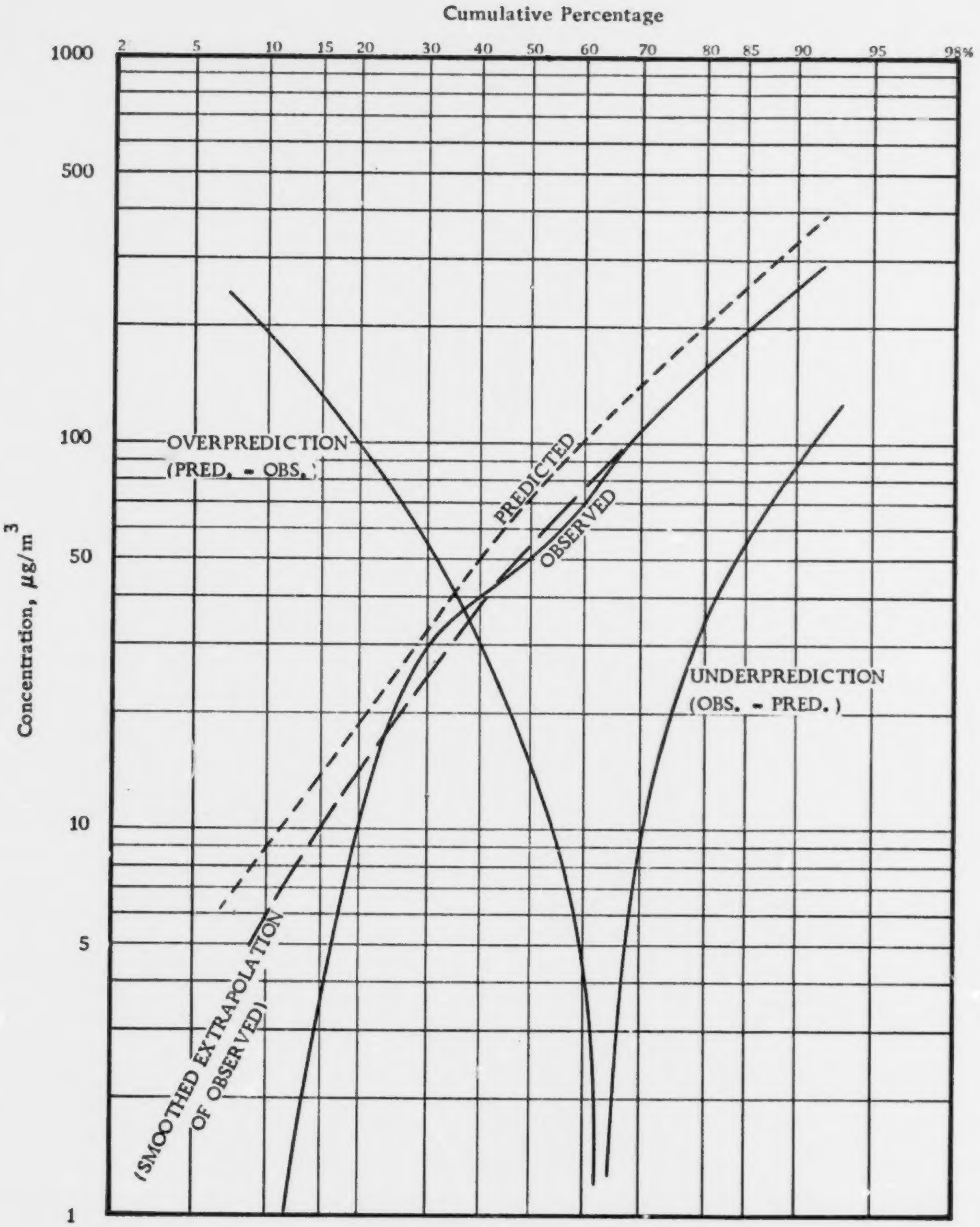


Figure 24. Frequency Distributions of Observed, Predicted and Observed-Minus-Predicted One-Hour Concentrations for Eight Chicago Stations Combined

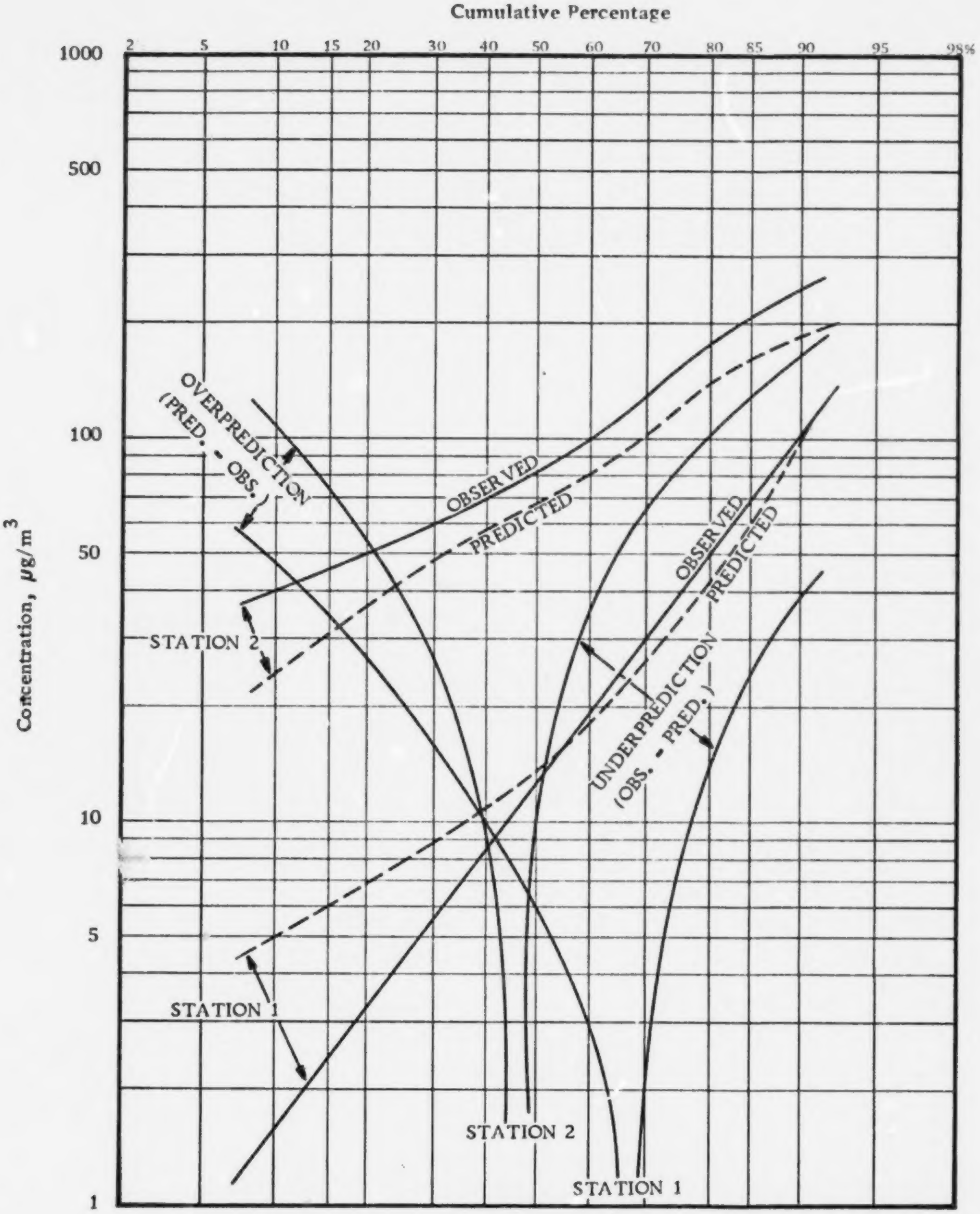


Figure 25. Frequency Distributions of Observed, Predicted and Observed-Minus-Predicted One-Hour Concentrations for Chicago Stations 1 and 2

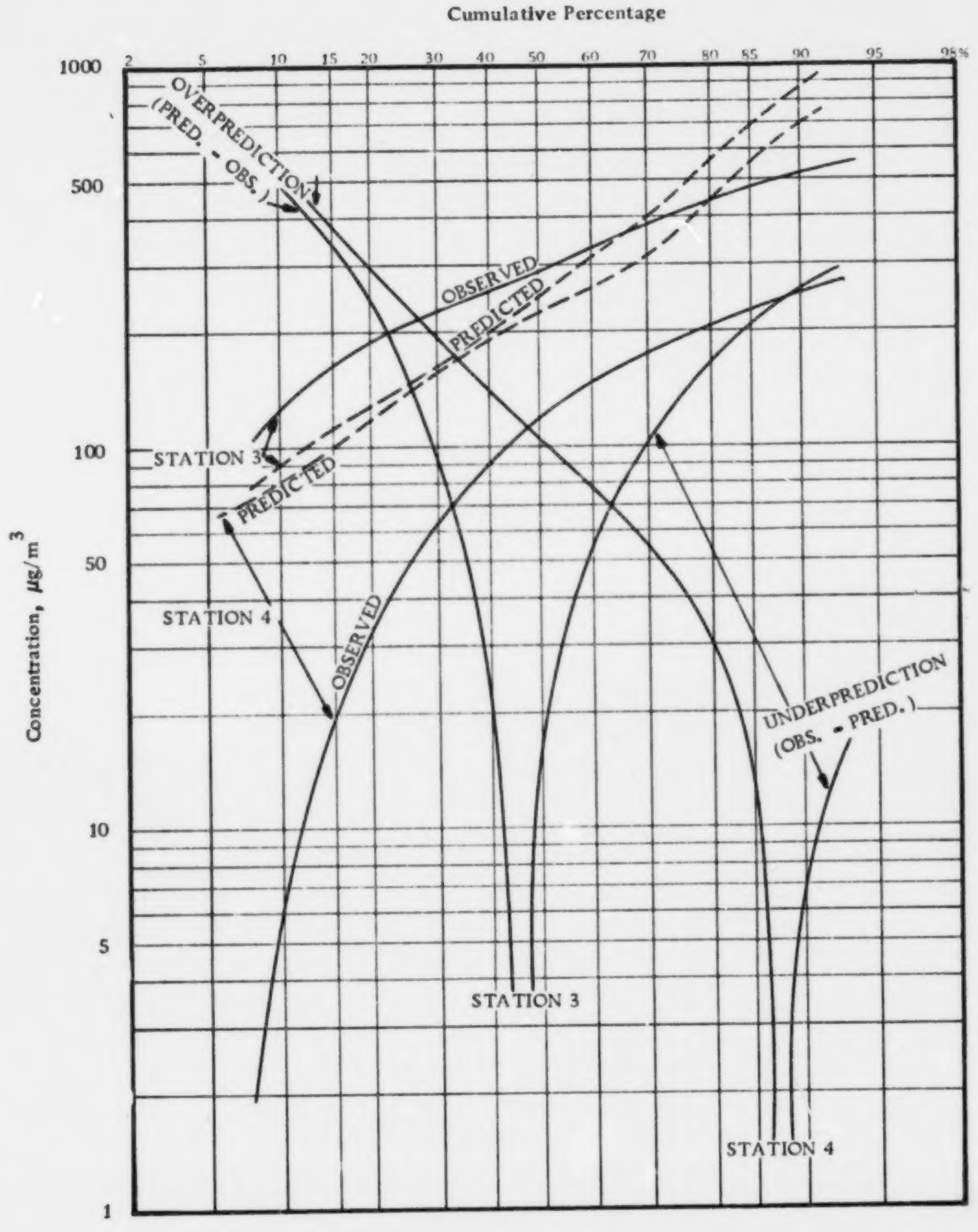


Figure 26. Frequency Distributions of Observed, Predicted and Observed-Minus-Predicted One-Hour Concentrations for Chicago Stations 3 and 4

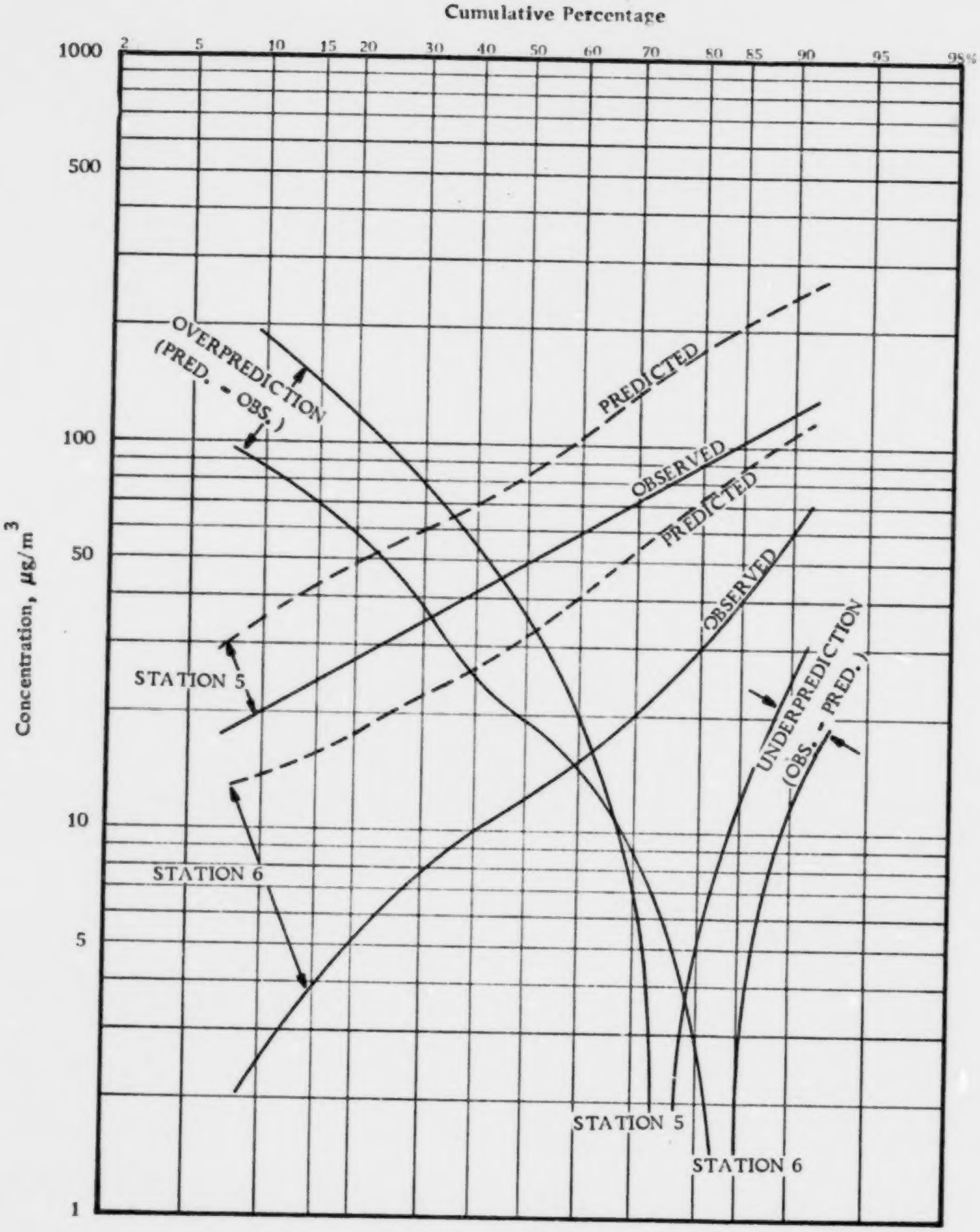


Figure 27. Frequency Distribution of Observed, Predicted and Observed-Minus-Predicted One-Hour Concentrations for Chicago Stations 5 and 6

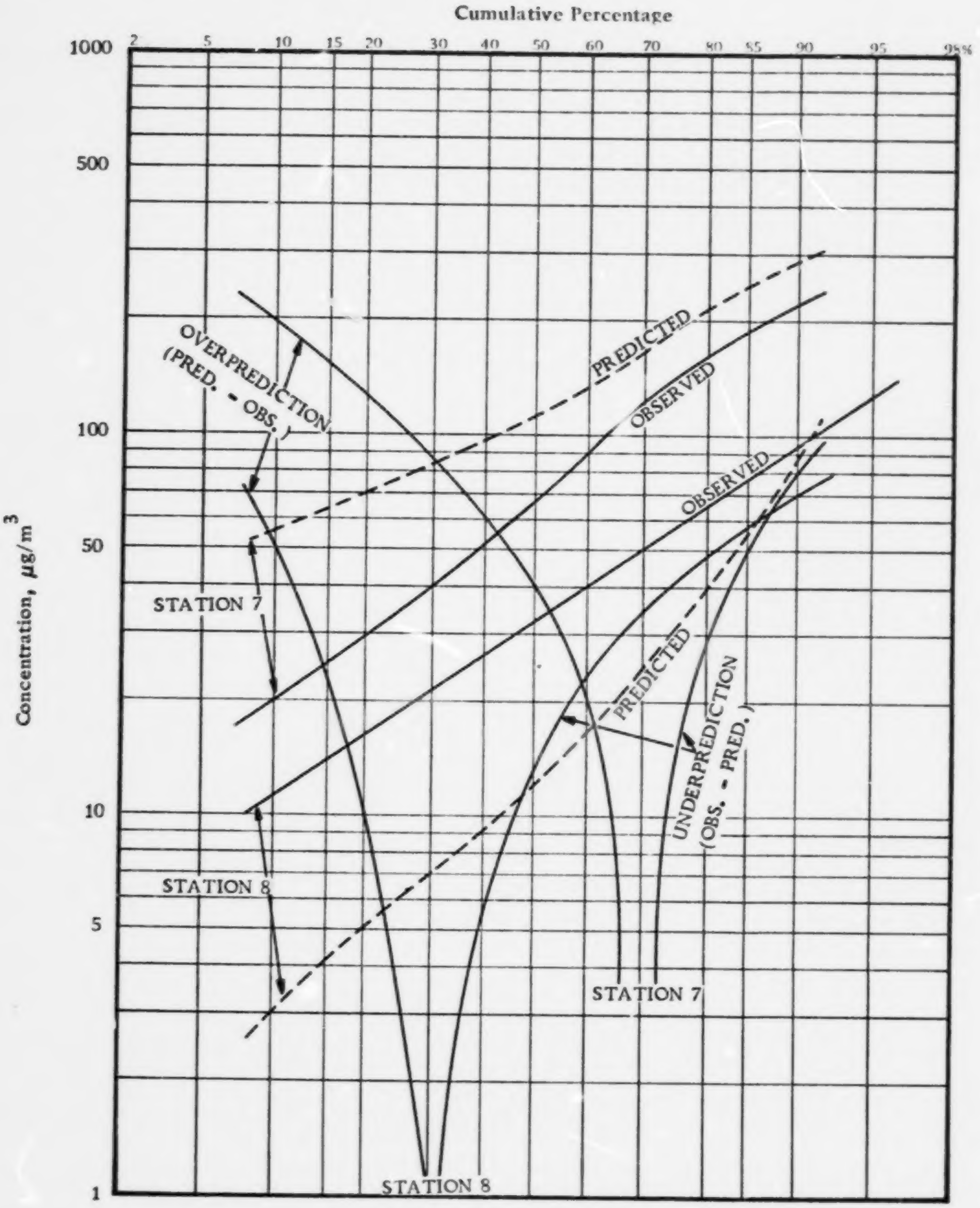


Figure 28. Frequency Distributions of Observed, Predicted and Observed-Minus-Predicted One-Hour Concentrations for Chicago Stations 7 and 8

to the observed frequency. Close correspondence between the predicted and observed frequency distributions is shown for stations 1, 2, and 3 in Figures 25 and 26. However, for all 8 stations the slopes of the curves for the two frequency distributions are similar. The frequency distributions of observed minus predicted values shown for each station in Figures 25 to 28 give a detailed breakdown of the wide variations which occur for single hour comparisons between predicted and observed values.

The predicted and observed mean concentrations for all 8 stations over the 31-day period are shown in Table 9 to be 145 and 96 $\mu g/m^3$, respectively. The standard deviations of hourly values were 232 and 117 $\mu g/m^3$, respectively. Figure 24 reflects the general tendency to overpredict for these data. The smoothed extrapolation of observed values shown in Figure 24 was constructed to attempt to account for threshold and sensitivity limitations of the monitoring equipment. However, the validation statistics in this analysis are based on the reported observations and do not reflect possible observation errors due to instrument limitations. Approximately 50 percent of all the predicted values were within 45 $\mu g/m^3$ of the observed values. This is in comparison with a mean value of 96 $\mu g/m^3$ and a median value of 50 $\mu g/m^3$. Approximately 73 percent of the predicted values were within 100 $\mu g/m^3$ of the observed values.

4.2.3 Very Light Wind Speed Situations and Model Validity with Variations in Wind Speed

It may be noted in Equations 28 and 29 that concentrations predicted by the Gaussian plume urban diffusion model are undefined for a wind speed of zero. An exception may occur if, as suggested by Roberts, et al., (1970), the diffusion parameters are treated as functions of time rather than distance.* Vectorially averaged wind speeds at a height of 20 meters were never less than 1.5 m/sec in the St. Louis data set. However, in the Chicago data set, several instances of nearly zero wind occurred, resulting in very large concentration predictions. As a result, it was decided to separate from the validation analysis all periods in which the wind speed was less than 1.0 m/sec and analyze them separately.

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* If the diffusion parameters σ_y and σ_z are treated as power functions of time, the substitution of distance divided by wind speed (x/u) for time will, for certain powers, result in an expression for concentration which approaches zero as wind speed approaches zero. The problem with this approach is that most experimental data suggest that the diffusion parameters are functions of distance rather than time. The use of time implies that the diffusion parameters are inversely proportional to a power of wind speed rather than directly proportional as is commonly observed in wind tunnel experiments.

In retrospect, an attempt was made to determine what should be done about situations with wind speeds less than 1.0 m/sec. One method contemplated was to extrapolate the trend of observed concentrations with wind speed averaged over all observations to eliminate the appropriate values for low wind speeds. Tables 10 and 11 show the relation between wind speed and observed short-term concentrations for locations in St. Louis and Chicago, respectively. The lowest wind speed class at each of the two sites contradicts the otherwise consistent inverse proportionality relationship. As a matter of interest, the predicted and observed minus predicted concentration relationships with wind speed are also shown. These results show that the model predicts a greater variation in concentration with wind speed than is reflected by the observations. If all the error were attributed to wind speed, the average overprediction error would be 50 percent or greater for wind speeds less than 2.5 m/sec for St. Louis and less than 4.0 m/sec for Chicago.

At present it appears that the model is inappropriate for predicting concentrations in very light wind situations (e.g., $u \leq 1.5$ m/sec). An alternative is to use the model to predict short-term concentrations for wind speeds in excess of 1.5 m/sec, and to use an empirical estimate to predict short-term concentrations for wind speeds less than, or equal to, 1.5 m/sec. An empirical estimate may be derived for a sampler location by first dividing all the concentrations observed during each short-term period (one or two hours) in which the mean wind speed is less than 1.5 m/sec by the average emission rate from all sources during each period.

Table 10. Observed, Predicted and Observed Minus Predicted Concentrations By Wind Speed Class for St. Louis Data

Wind Speed Class (m/sec)	Two Hour Concentrations ($\mu g/m^3$)						Number of Cases
	Observed		Predicted		Obs. - Pred.		
	Mean	Std. Dev.	Mean	Std. Dev.	Mean	St. Dev.	
1.5	171	142	659	618	-488	618	30
$1.5 < u \leq 2.0$	245	200	343	250	- 98	229	110
$2.0 < u \leq 2.5$	208	195	325	267	-117	281	415
$2.5 < u \leq 3.0$	197	171	257	238	- 60	241	660
$3.0 < u \leq 4.0$	178	162	198	210	- 21	223	1781
$4.0 < u \leq 5.0$	154	140	143	151	11	169	1993
$5.0 < u \leq 6.0$	136	135	113	115	24	142	1800
$6.0 < u \leq 8.0$	138	180	88	93	50	164	1966
$8.0 < u \leq 10.0$	104	112	71	68	33	105	600
$10.0 < u$	96	106	53	50	43	89	65

Table 11. Observed, Predicted and Observed Minus Predicted Concentrations By Wind Speed Class for Chicago Data

Wind Speed Class (m/sec)	Number of Cases	One Hour Concentrations ($\mu g/m^3$)					
		Observed		Predicted		Obs. - Pred.	
		Mean	St. Dev.	Mean	St. Dev.	Mean	St. Dev.
$1.0 < u \leq 1.5$	88	116	117	430	385	-314	356
$1.5 < u \leq 2.0$	238	149	143	364	400	-215	359
$2.0 < u \leq 2.5$	279	125	135	276	484	-151	450
$2.5 < u \leq 3.0$	462	113	123	185	267	- 72	230
$3.0 < u \leq 4.0$	1089	107	128	165	211	- 57	169
$4.0 < u \leq 5.0$	1117	95	117	116	147	- 22	124
$5.0 < u \leq 6.0$	929	91	112	119	159	- 28	131
$6.0 < u \leq 8.0$	715	70	94	72	121	- 2	126
$8.0 < u \leq 10.0$	466	55	65	53	50	1	59
$10.0 < u$	24	59	68	38	35	22	46

The mean of these computed ratios times the emission rate $Q_j(t)$ for a period (t) of interest provides an empirically estimated concentration $x_j(t)$ as indicated by following equation:

$$x_j(t) = Q_j(t) \frac{1}{N} \sum_{i=1}^{N} \frac{x_i}{Q_i} \tag{40}$$

If observations are not available, an empirical estimate can be obtained from the model by using a wind speed of 4 m/sec to approximate the light wind speed situation and averaging the concentrations predicted for each of the sixteen major compass points as a wind direction. The selection of 4 m/sec for a wind speed is based on the validation results which show that for St. Louis the mean concentration observed with wind speeds of 1.5 m/sec lies between the predictions for wind speeds of 3 to 4 m/sec and those for 4 to 5 m/sec; for Chicago the mean concentration for wind speeds of 1.0 to 1.5 m/sec equal those predicted for wind speeds of 4 to 5 m/sec.

The cause of the trend from underprediction to overprediction with decreasing wind speed is not clear. It may be associated with inadequate estimates of the diffusion parameters σ_z (and σ_y to a lesser extent) and with inadequate accounting of the effect of wind speed in emission rates. At present no dependence on wind speed is considered for emission rates. For example, the fuel consumption rate for space heating is presently taken to be a function of temperature; however, it is also affected by wind speed. During high wind speeds, greater fuel consumption occurs than is predicted which results in higher emission rates and higher observed concentrations than are predicted. Similarly, during light wind speeds, lower fuel consumption rates occur which result in lower observed concentrations than are predicted. The dependence of diffusion parameters on wind speed is presently taken to be one in which the parameters vary directly with the product of wind speed and time (i.e., the parameters are functions of travel distance). While considerable support for this relationship has been reported from tracer experiments in flat, open country, it may be less appropriate in an urban area.

The mean prediction error (i.e., mean one- or two-hour observed concentration minus predicted concentration at each sample location averaged over all locations and all observing periods) is less than 50 percent of the mean observed concentration for wind speed classes in excess of 2.5 m/sec in St. Louis and wind speed classes in excess of 4 m/sec in Chicago. For wind speeds of 1.5 m/sec in St. Louis and a wind speed class of 1.0 to 1.5 m/sec in Chicago the mean prediction error is greater than twice the mean observed concentration in both St. Louis and Chicago.

4.2.4 Summary and Conclusions for Short-Term Concentrations

The Chicago error distributions are not greatly different from those observed for St. Louis. Thus, although the overall distribution of predicted values for Chicago seems to be biased to the high side, relative to the distribution of observed values, the magnitude of the errors between predicted and observed values is not much greater. On this basis the validity of the model has been summarized in terms of the frequency distribution of absolute errors (predicted minus observed concentration) associated with the results of this study. A tabulation of error limits, and the percentage of the comparisons between predicted and observed concentrations which lie within each limit, is given in Table 12 for the St. Louis and Chicago results. The values entered in this table are obtained from Figures 17 and 24 by subtracting the cumulative percentage of overpredictions from the cumulative percentage of underpredictions which correspond to a concentration error range.

Table 12. Comparison of Error Distributions for Two-Hourly St. Louis and Hourly Chicago Validation Calculations

Range of Predicted Minus Observed Concentration μg/m^3	% of Comparisons Within Error Limits	
	St. Louis (Mean Observed Concentration = 154 μg/m^3)	Chicago (Mean Observed Concentration = 96 μg/m^3)
± 5	8	8
± 10	15	17
± 20	25	30
± 50	46	53
+100	65	73
±150	76	82

As a concluding comment on this portion of the analysis, it is noted that, except for wind speed discussed in the preceding section, no single factor was shown to consistently affect the results. The prediction errors appear to result from a variety and random sequence of errors in both the observations and the model parameters. Factors which are particularly uncertain are the accuracy of an individual sampler observation for a short-term period (especially for the Chicago data where duplicate sampling was not available), the hourly emission rate estimates which may conta[illegible] temperature or time of day biases which are systematic over the entire city, and estimates of diffusion parameter values (σ_y and σ_z) which cannot clearly be delineated by atmospheric stability measurements. A more complete discussion of the effect of model inputs on model predictions is given in Section 5.0 on sensitivity analysis.

If the validity of the model is judged on the basis of its ability to reproduce the observed frequency distribution of short term concentrations over a long term period, the model gives satisfactory results when the combined frequency distribution for several observing locations is considered. Comparisons of predicted and observed frequency distributions at individual locations are more variable. Another basis for judging validity is to compare the standard deviation of observed minus predicted concentrations (root-mean-square-error) for model predictions with that for empirically derived predictions. On this basis, Marsh and Withers (1969) concluded from a model validation study conducted with data from Reading, England, that empirical models are more satisfactory than the Gaussian plume type of dispersion model for predicting SO_2 concentrations from area sources. However, the model approach is more general, does not require empirical adjustment, and provides greater confidence for extrapolation to unobserved conditions.

It is concluded that, although one-hour or two-hour predicted SO_2 concentrations show large deviations from observed values from hour to hour, the frequency distribution of observed values over a month or a season are closely approximated by the frequency distribution of predicted values. This conclusion is based on the use of routine airport and radiosonde meteorological observations for estimating diffusion parameters and the mixing ceiling, multiple (three or more) continuous measurements for measuring hourly averages of wind speed and direction, and moderately detailed emission inventory data (e.g., including annual space heating and processing fuel requirements and stack characteristics of large fuel users, hourly power outputs of electricity generating plants).

4.3 RESULTS OF LONG-TERM CALCULATIONS

In the preceding section the validity of model predictions of hourly (and two-hourly) concentrations, and the distribution of these concentrations over a month, or a season, were examined. In this present section, the validity of the model for long-term mean prediction is examined. As with the short-term concentrations the long-term mean concentration data include a moderately detailed emission inventory from which hourly estimates of emission rates were derived, routine airport weather observations to estimate atmospheric stability, radiosonde observations to estimate mixing ceiling heights, and the mean of several continuous wind speed and direction averages (three locations for St. Louis, eight for Chicago). Also, in view of the computations required to derive a mean by averaging a large number of one-hour values, the use of a statistical sampling plan to reduce the computations is presented in Section 4.3.2. This approach provides a method of treating many variables in the model (not just three) without unduly adding to the computational burden. Finally, results obtained in this study are compared with other long-term validation study results.

4.3.1 Validation Results

Figure 29 shows the mean of predicted and observed two-hour concentrations for the 1964-65 winter season consisting of December, January and February at 10 stations in the St. Louis area. The means show relatively good agreement with observed seasonal means. A root-mean-square-error (RMSE) of 56 $\mu g/m^3$ was observed compared to an overall mean of 154 $\mu g/m^3$. Furthermore, the correlation between predicted and observed seasonal means is quite good, as shown in Figure 30 (representing a regression of observed values on predicted with a slope of 0.98 and intercept of slightly less than zero). The correlation coefficient of 0.675 indicates that the regression line accounts for about 46 percent of the observed variance.

The mean of hourly concentrations for Chicago Telemetering Air Monitor (TAM) stations for the month of January 1967 is shown in Figure 31. The RMSE for monthly mean concentration at eight stations was 78 $\mu g/m^3$ compared to an overall observed mean of 96 $\mu g/m^3$. Figure 32 shows the correlation between predicted and observed monthly mean values for the eight stations. The slope of the regression line is 0.63 and the intercept is 4.9. The results suggest a tendency of the model to overpredict. In the above comparisons, cases in which the wind speed was less than 1.0 meter per second were not included. For such low wind speeds, local circulation effects will dominate over a general transport phenomenon such as is inherent in a steady-state Gaussian plume model.

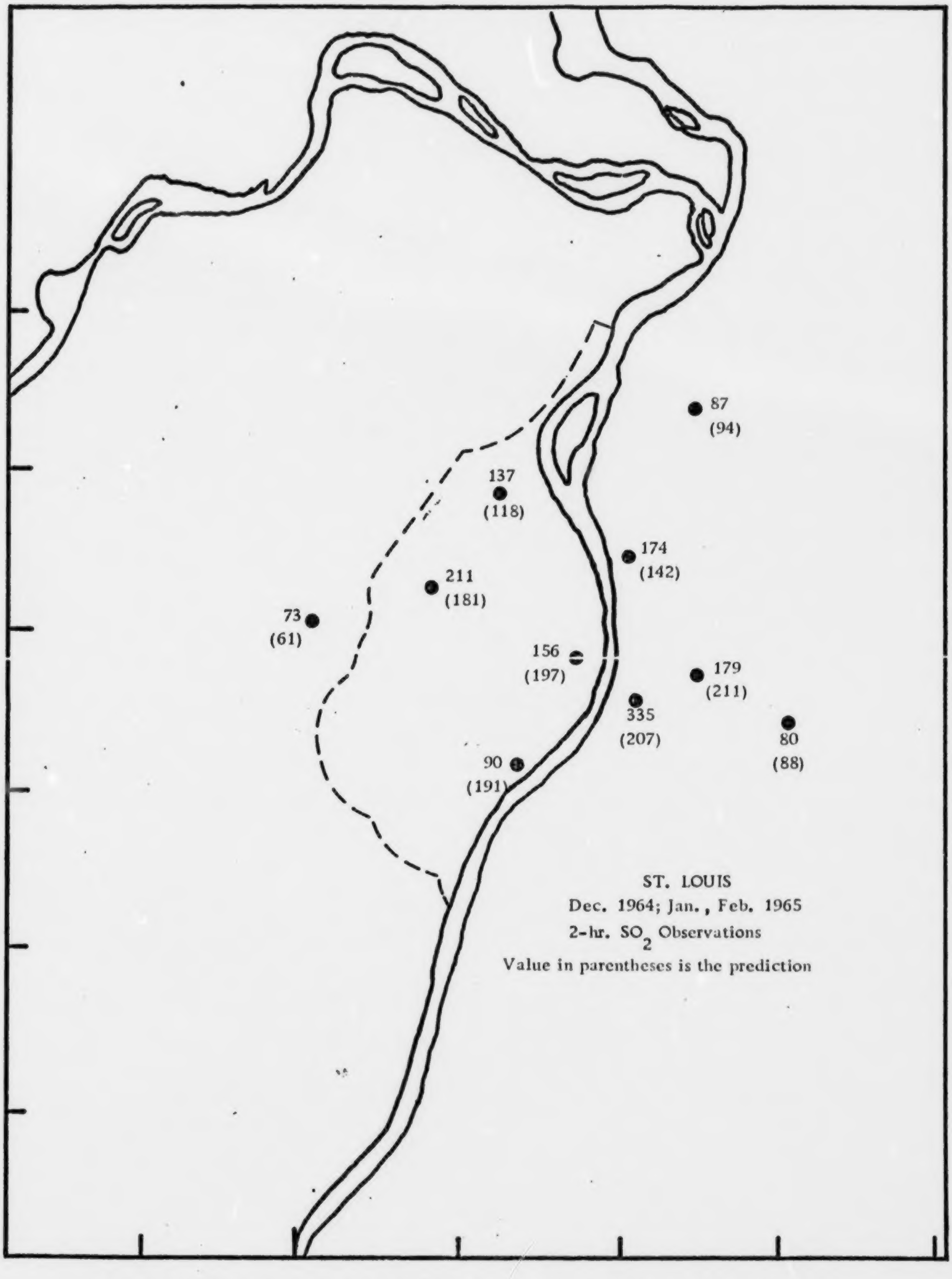

87
(94)
137
(118)
174
(142)
211
(181)
73
(61)
156
(197)
179
(211)
335
(207)
80
(88)
90
(191)
ST. LOUIS
Dec. 1964; Jan., Feb. 1965
2-hr. SO_2 Observations
Value in parentheses is the prediction

Figure 29. Observed and Predicted Seasonal Mean Concentrations for 10 St. Louis Stations

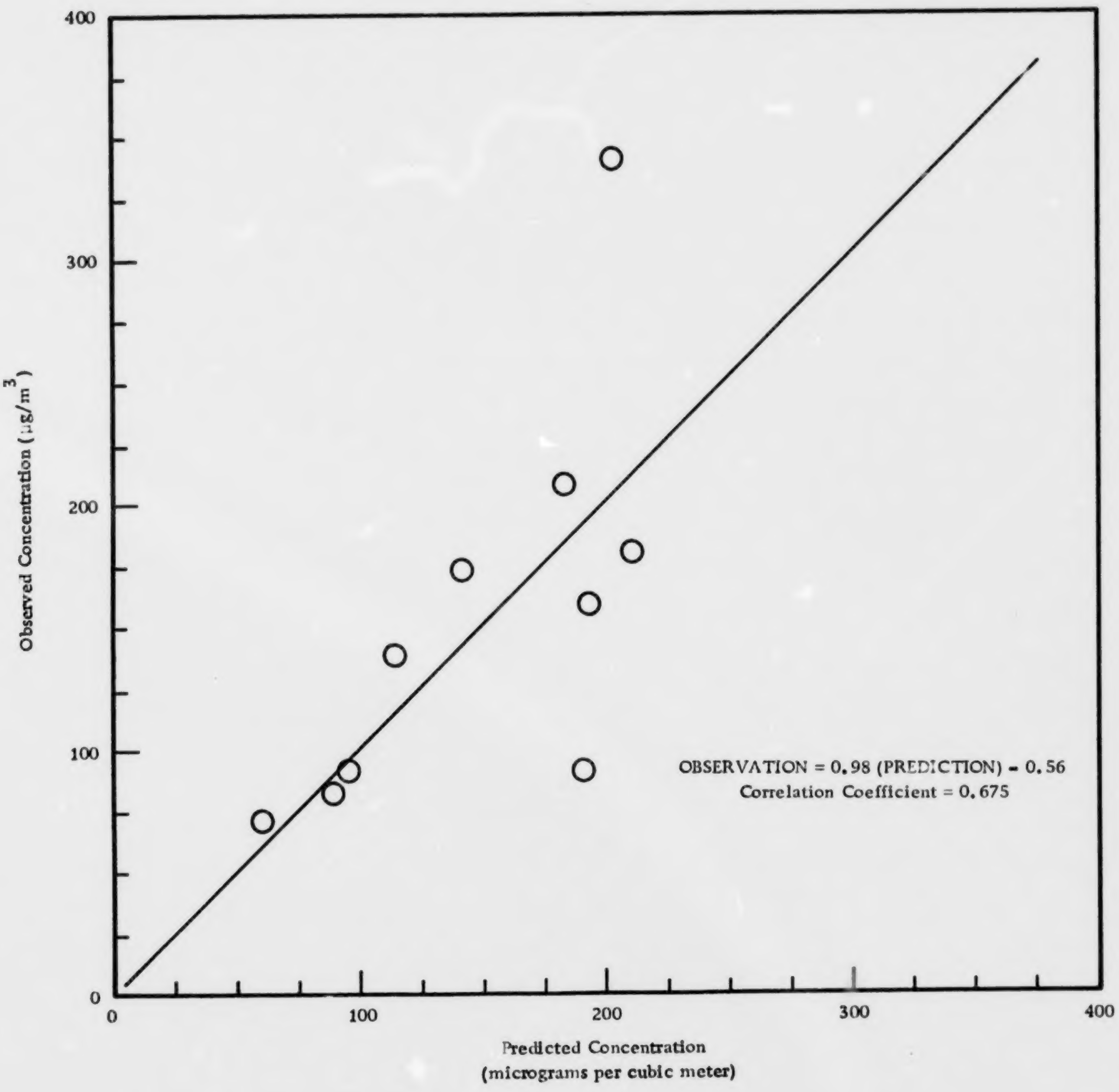
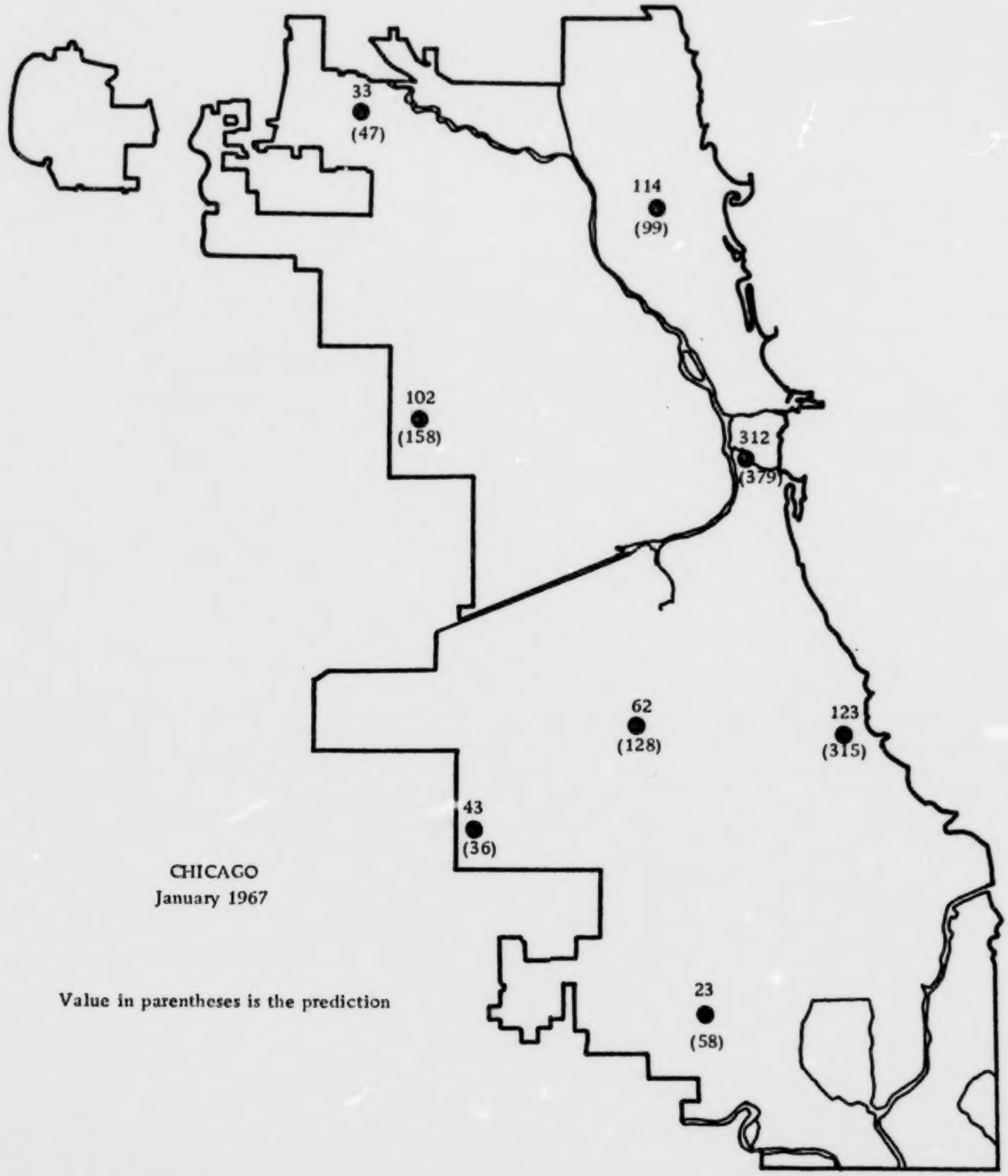


Figure 30. Regression Analysis of Seasonal Mean Concentrations for 10 St. Louis Stations (Winter 1964-65)


33
(47)
114
(99)
102
(158)
312
(379)
62
(128)
123
(315)
43
(36)
23
(58)

CHICAGO
January 1967

Value in parentheses is the prediction

Figure 31. Observed and Predicted Mean Monthly Concentrations for Eight Chicago Stations

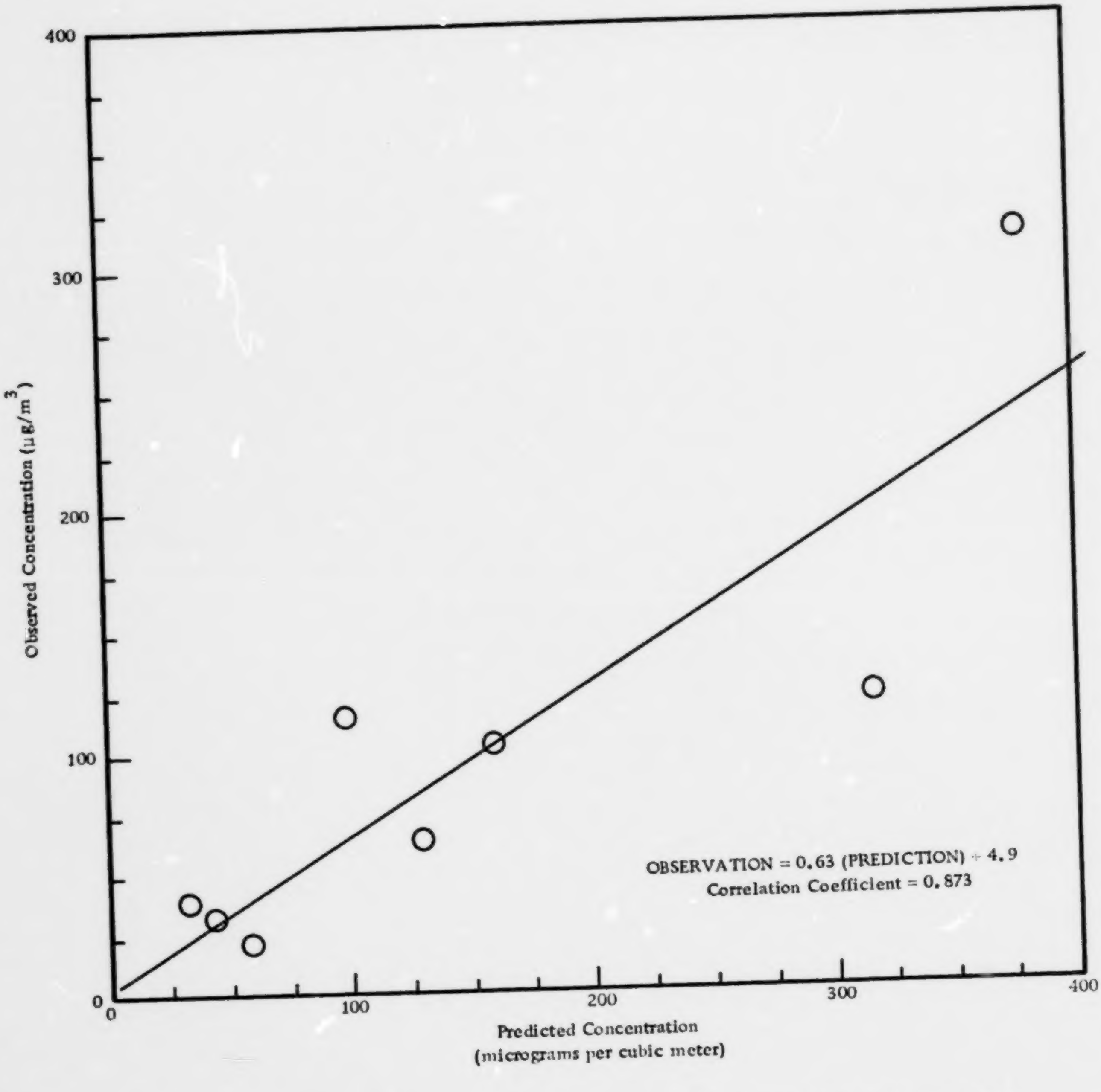


Figure 32. Regression Analysis of Monthly Mean Concentrations for Eight Chicago Stations (January 1967)

The combined long-term RMSE for individual station means at both locations was 68 $\mu g/m^3$ compared to an overall mean of 128 $\mu g/m^3$. This shows that the overall RMSE is about one-half of the overall mean. The median observed minus predicted concentration for the two locations was -11.5 $\mu g/m^3$. In addition the long-term mean was overpredicated at 11 stations and underpredicted at seven stations. These results indicate a tendency to overestimate observed concentrations more often than to underestimate.

4.3.2 Use of Sampling Plan

In most previous approaches to computing long-term concerntrations it has been assumed that emission rates are independent of meteorological conditions, and the long-term average concentrations were calculated using a mean emission rate. This assumption was necessitated by the lack of data available to estimate diurnal variations. In the more detailed approach used in this study all hourly concentrations within a long-term period are calculated to determine the long-term mean and the frequency distribution of short-term concentrations. This requires a considerable computational burden. It is desirable to introduce a computational procedure which does not bias the correlation between emission rates and meteorological conditions and does not require excessive computation time. An approach to reducing the running time by statistical sampling of a calendar-time-oriented input set has been developed (Hansen et al. 1953).* It amounts to deriving a mean and frequency distribution of calculated concentrations using only a sampled set of inputs. For example, if every other hour is sampled, the long-term concentration may still be obtained and the computations are reduced by a factor of 2. If every sixth hour is used, computations are reduced by a factor of 6, etc. In the proposed plan the hours are statistically sampled by randomly selecting the first hour of the first day in the set, and selecting additional hours which are one sample increment away from the selected hour, as follows: The first hour is incremented by one for each succeeding day in the calendar period. Thus, if the sample increment is six hours and the first selected hour is hour 1, hours 1, 7, 13 and 19 will be selected from the first day; hours 2, 8, 14 and 20, from the second day; etc.

In order to test the validity of the use of various sampling intervals, the sampling plan was applied to the St. Louis data at each of the 10 stations for which hourly calculations had been made for the months of December 1964, January and February 1965. The mean, standard deviation and deciles of hourly concentrations obtained with statistical sampling intervals of 2, 4, 6, 8, 12 and 24 hours are listed in Table 13 for station number 3. Results for the other nine stations are shown in Tables 14 through 22. The largest deviation of a decile concentration for a 24-hour sampling interval, from that obtained with a one-hour sampling interval, was 25 percent of the one-hour decile value. In absolute magnitude the greatest deviation was 601 $\mu g/m^3$ compared to 513 $\mu g/m^3$ for the one-hour 90 percent decile at station number 12. The results show that, except for the single highest value, the entire frequency distribution of concentrations can be reasonably reproduced using a 24-hour interval between sampled periods. Table 23 shows the mean, standard deviation and deciles for all hourly station concentrations combined. Except for the extreme maximum the largest difference between a mean two-hour decile concentration and a decile concentration from the 24-hour sampling interval is 17 $\mu g/m^3$ for the 90th percentile. This is about 10 percent of the mean value of 2-hour averages of 151 $\mu g/m^3$, and about 5 percent of the 90 percentile value of 363 $\mu g/m^3$. In the view of the uncertainties in the model predictive accuracy on an hour-by-hour basis shown by the comparisons between predicted and observed concentrations, the small errors in constructing frequency distributions by using the selective 24-hour sampling plan illustrated above do not seem to be significant.

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*The type of sampling used here is known as proportionate stratified sampling. The following excerpt from page 121 of the cited reference defines the term: ".... the elements (sampling units) of the population are divided into groups, referred to as strata, such that each element is contained in one and only one stratum. The sample is then chosen by selecting a simple random sample of elements from each stratum. The sampling fraction may vary from stratum to stratum or may be uniform in all strata. If the sampling fraction is uniform the sampling plan is referred to as proportionate stratified sampling."

The sampling units are hourly concentration values. The strata are the hours of the day and the days of the week. The sampling plan ensures that the sampling fraction is uniform over the strata. The method of taking every n-th observation is not strictly random but is equivalent to it unless there is a periodicity of length n in the data. It is assumed that there is no periodicity for the values of n used here.

Table 13. Mean, Standard Deviation and Deciles of Predicted Hourly Concentrations Over Winter Season for St. Louis Station #3

	Sampling Interval, Hours						
	1	2	4	6	8	12	24
No. of Cases	2122	1060	530	351	267	176	86
Mean, $\mu g/m^3$	195	191	193	195	190	200	188
Std. Dev., $\mu g/m^3$	205	171	173	180	172	187	170
Deciles ($\mu g/m^3$):							
0 (a)	10	10	10	10	17	10	18
10	53	53	51	52	51	53	51
20	71	72	70	72	68	70	64
30	87	87	86	88	82	87	82
40	105	106	107	105	102	109	103
50	128	127	128	126	123	131	118
60	163	156	162	155	150	156	146
70	211	208	214	207	201	208	202
80	289	291	296	301	296	296	270
90	430	429	434	446	434	449	409
100	5019	1195	1195	1195	1025	1195	1025

(a) Lowest Value

Table 14. Mean, Standard Deviation and Deciles of Predicted Hourly Concentrations Over Winter Season for St. Louis Station #4

	Sampling Interval, Hours						
	1	2	4	7	9	12	24
No. of Cases	2122	1060	530	351	267	176	86
Mean, $\mu g/m^3$	143	145	150	139	150	138	133
Std. Dev., $\mu g/m^3$	204	211	227	150	195	151	154
Deciles ($\mu g/m^3$):							
0 (a)	8	8	10	10	10	10	10
10	22	22	21	21	21	19	19
20	31	31	30	29	28	29	29
30	44	44	43	44	44	37	37
40	58	56	58	57	61	54	54
50	80	79	80	81	81	81	81
60	110	103	107	110	111	114	100
70	151	152	146	161	144	153	136
80	215	215	233	215	215	220	202
90	325	335	335	330	355	330	294
100	4254	3371	3371	979	1428	979	979

(a) Lowest Value

Table 15. Mean, Standard Deviation and Deciles of Predicted Hourly Concentrations Over Winter Season for St. Louis Station #10

	Sampling Interval, Hours						
	1	2	4	6	8	12	24
No. of Cases	2122	1060	530	351	267	176	86
Mean, $\mu g/m^3$	208	208	209	205	204	194	207
Std. Dev., $\mu g/m^3$	182	184	182	182	181	165	171
Deciles ($\mu g/m^3$):							
0(a)	11	14	14	15	14	15	15
10	44	45	47	47	47	47	35
20	69	70	70	71	71	70	56
30	96	95	94	97	88	88	79
40	120	119	115	117	113	112	112
50	149	145	149	145	146	141	152
60	192	188	190	184	190	171	190
70	243	243	253	236	243	231	278
80	318	319	321	304	302	301	321
90	448	436	432	404	393	393	400
100	1626	1626	1154	1626	1054	999	872

(a) Lowest Value

Table 16. Mean, Standard Deviation and Deciles of Predicted Hourly Concentrations Over Winter Season for St. Louis Station #12

	Sampling Interval, Hours						
	1	2	4	6	8	12	24
No. of Cases	2122	1060	530	351	267	176	86
Mean, μg/m^3	220	217	224	221	234	220	250
Std. Dev., μg/m^3	239	232	245	256	273	260	309
Deciles (μg/m^3):							
0$^{(a)}$	10	11	11	12	11	17	17
10	37	37	38	37	40	36	36
20	53	52	53	52	59	50	60
30	72	72	71	70	76	66	81
40	101	101	100	100	104	97	100
50	136	134	132	129	131	132	138
60	182	179	180	176	178	175	183
70	244	243	251	230	243	238	270
80	335	326	338	315	319	303	313
90	513	487	506	490	565	463	601
100	2211	2070	2070	2070	2070	2070	2070

(a) Lowest Value

Table 17. Mean, Standard Deviation and Deciles of Predicted Hourly Concentration Over Winter Season for St. Louis Station #15

	Sampling Interval, Hours						
	1	2	4	6	8	12	24
No. of Cases	2122	1060	530	351	267	176	86
Mean, $\mu g/m^3$	123	120	118	127	113	133	117
Std. Dev., $\mu g/m^3$	139	128	127	144	120	158	139
Deciles ($\mu g/m^3$):							
0 (a)	3	7	7	7	9	7	9
10	22	22	22	22	20	21	22
20	31	32	32	32	30	29	30
30	42	41	42	41	41	39	37
40	57	57	58	54	60	57	58
50	78	77	78	76	78	75	78
60	101	98	96	102	96	97	95
70	132	129	126	137	115	137	113
80	182	176	174	185	163	182	152
90	274	269	262	284	253	304	223
100	1370	931	931	931	931	931	931

(a) Lowest Value

Table 18. Mean, Standard Deviation and Deciles of Predicted Hourly Concentration Over Winter Season for St. Louis Station #17

	Sampling Interval, Hours						
	1	2	4	6	8	12	24
No. of Cases	2122	1060	530	351	267	176	86
Mean, $\mu g/m^3$	181	181	181	178	180	185	201
Std. Dev., $\mu g/m^3$	172	180	172	152	166	166	189
Deciles ($\mu g/m^3$):							
0 (a)	9	9	9	9	9	9	9
10	48	46	45	47	45	53	55
20	67	65	64	64	65	65	73
30	83	82	80	80	82	80	82
40	101	101	102	97	104	102	113
50	125	127	133	127	126	137	137
60	155	155	159	157	156	157	166
70	203	201	203	208	201	201	223
80	260	260	260	271	260	269	272
90	383	378	369	380	381	393	380
100	1759	1759	1623	1016	1252	1016	1016

(a) Lowest Value

Table 19. Mean, Standard Deviation and Deciles of Predicted Hourly Concentration Over Winter Season for St. Louis Station #23

	Sampling Interval, Hours						
	1	2	4	6	8	12	24
No. of Cases	2122	1060	530	351	267	176	86
Mean, $\mu g/m^3$	185	189	188	184	181	193	216
Std. Dev., $\mu g/m^3$	260	270	251	247	235	269	288
Deciles ($\mu g/m^3$):							
0 (a)	5	5	7	5	7	7	8
10	15	14	14	14	14	13	13
20	24	24	24	24	23	24	23
30	42	42	43	42	42	47	35
40	60	58	62	58	61	62	63
50	88	84	92	81	89	93	103
60	127	126	130	116	130	116	140
70	177	187	189	187	173	190	264
80	283	289	287	291	283	291	313
90	483	483	460	460	460	494	519
100	3215	3215	1614	1614	1614	1614	1614

(a) Lowest Value

Table 20. Mean, Standard Deviation and Deciles of Predicted Hourly Concentrations Over Winter Season for St. Louis Station #28

	Sampling Interval, Hours						
	1	2	4	6	8	12	24
No. of Cases	2122	1060	530	351	267	176	86
Mean, $\mu g/m^3$	94	92	96	92	106	97	115
Std. Dev., $\mu g/m^3$	174	165	180	163	210	183	225
Deciles ($\mu g/m^3$):							
0 (a)	1	1	1	1	1	1	1
10	2	2	2	3	2	2	2
20	5	5	5	5	4	4	4
30	9	9	9	9	9	9	9
40	15	14	14	15	14	14	12
50	25	25	24	23	25	23	24
60	45	44	44	41	47	37	33
70	81	81	76	82	71	63	63
80	146	144	139	139	134	133	125
90	246	245	237	232	259	234	280
100	2344	1457	1457	1117	1457	1117	1117

(a) Lowest Value

Table 21. Mean, Standard Deviation and Deciles of Predicted Hourly Concentrations Over Winter Season for St. Louis Station #33

	Sampling Interval, Hours						
	1	2	4	6	8	12	24
No. of Cases	2122	1060	530	351	267	176	86
Mean, $\mu g/m^3$	60	59	58	54	57	60	69
Std. Dev., $\mu g/m^3$	105	102	99	78	97	89	112
Deciles ($\mu g/m^3$):							
0 (a)	1	1	1	1	1	1	1
10	6	6	6	6	5	5	5
20	9	9	9	9	9	9	9
30	14	14	14	14	13	14	14
40	19	19	19	19	17	19	21
50	25	26	26	26	24	27	27
60	34	34	35	35	32	38	36
70	51	51	52	55	52	61	57
80	76	74	74	81	74	91	91
90	144	136	132	132	125	138	140
100	1235	1180	1180	741	846	741	741

(a) Lowest Value

Table 22. Mean, Standard Deviation and Deciles of Predicted Hourly Concentrations Over Winter Season for St. Louis Station #36

	Sampling Interval, Hours						
	1	2	4	6	8	12	24
No. of Cases	2122	1060	530	351	267	176	86
Mean, $\mu g/m^3$	93	93	98	87	99	79	86
Std. Dev., $\mu g/m^3$	151	156	164	143	174	121	119
Deciles ($\mu g/m^3$);							
0 (a)	1	2	2	2	2	2	3
10	9	9	9	9	9	9	11
20	15	15	13	15	14	14	17
30	20	20	20	19	19	20	20
40	27	27	26	26	26	26	26
50	37	37	36	34	36	34	34
60	54	54	55	50	48	45	44
70	77	75	86	71	83	73	96
80	118	114	118	110	122	109	127
90	222	221	239	191	220	165	191
100	1295	1295	1213	933	1213	891	686

(a) Lowest Value

Table 23. Mean, Standard Deviation and Deciles of Predicted Hourly Concentrations Over Winter Season for Ten St. Louis Stations

	Two-Hour Averages	Sampling Interval, Hours					
		2	4	4	4	12	24
No. of Cases	9420	10600	5300	3510	2670	1760	860
Mean, $\mu g/m^3$	151	149	151	148	152	150	158
Std. Dev., $\mu g/m^3$	179	193	195	184	196	190	206
Deciles ($\mu g/m^3$):							
0 (a)	1	1	1	1	1	1	1
10	16	13	13	13	13	13	14
20	29	26	26	25	25	25	25
30	48	41	42	41	41	42	41
40	67	60	62	61	62	61	62
50	91	84	85	85	85	85	87
60	122	114	114	114	114	115	118
70	168	157	159	157	156	156	160
80	235	231	237	229	229	234	247
90	363	365	365	369	361	376	380
100	3579	3371	3371	2070	2070	2070	2070

(a) Lowest Value

Table 24 summarizes the increasing uncertainty associated with increasing the sampling interval. The root-mean-square-error (RMSE) in mean long-term (seasonal) concentrations at a single station for various sampling intervals was calculated by comparing the concentration means with sampling to concentration means without sampling at 10 stations. The increasing size of the RMSE with increasing sampling interval indicates that one hour sampled out of every 24 is as large a sampling as should be used in treating a season.

Table 24. Summary of Accuracy of Sampling Intervals for Estimating Distribution of Predicted Concentrations Over a Season

Sampling Interval, Hours	Root Mean Square Error (RMSE),$^{(a)}$ $\mu g/m^3$	Mean, $\mu g/,^3$
1	--	150
2	2.43	150
4	3.70	152
6	3.58	148
8	7.69	151
12	7.94	150
24	16.43	158

(a) $(RMSE)_j = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_{1,i} - x_{j,i})^2}$

N = No. of Stations (10)

j = Sampling Interval

$X_{j,i}$ = Seasonal Mean Concentration for i th Station with Sampling Every Hour

$X_{1,i}$ = Seasonal Mean Concentration for i th Station with Sampling Every Hour

4.3.3 Comparisons with Other Studies

Comparison of the results with other studies suggests that the use of variations in emission rates improves the prediction of daily or seasonal concentrations of SO_2. Two examples of calculated SO_2 concentrations from previous studies using mean daily or seasonal emission rates and observed SO_2 concentrations have been reviewed in connection with this point. It may be noted that in both examples the investigators suggested the need to treat the variability in emission rates. The first example derived from Clarke (1964), is shown in Figure 33 and illustrates the distribution of mean daily

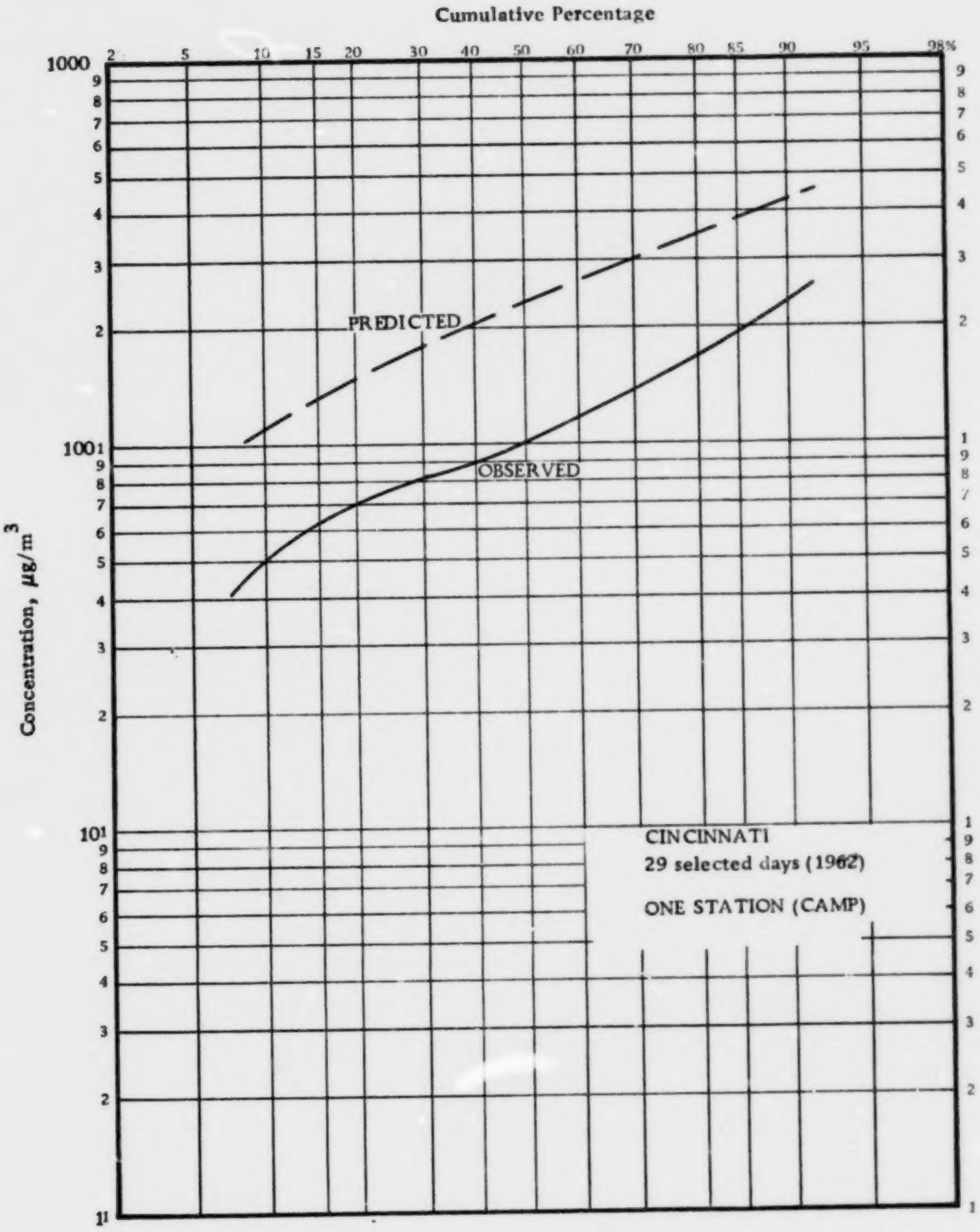


Figure 33. Frequency Distributions of Daily Mean Observed and Predicted Concentrations (from Clarke, 1964) Using Diurnal Mean Emission Rates

concentrations of SO_2 at the Cincinnati CAMP station for 29 selected days. The predicted values were generated using mean daily emission rates and are generally about twice the observed values. The second example was derived from Calder (1970). Figure 34 shows observed and predicted (in parenthesis) mean seasonal concentrations of SO_2 for 10 stations in St. Louis. The ratio of predicted to observed concentration varies from 2.6 to 4.3 which shows the general overprediction. The climatological mean concentrations were computed by summing the concentrations associated with combinations of six wind speeds, 16 wind directions, and six stability categories with each combination weighted according to its relative frequency of occurrence; the diffusion parameters used in these calculations are the Pasquill-Gifford parameters based on stability indexes derived using Turner's adaptation of Pasquill's definitions. The model assumes a mean climatological mixing ceiling.

Figure 35 shows the observed and predicted frequency distribution of seasonal concentrations. The frequency distribution of observed values is overpredicted by a factor of 3. Figure 36 shows a graphical comparison of the results for the 10 stations. It also shows a regression line of observed concentrations on predicted concentrations determined by Calder for 40 stations. This figure shows that the 10 stations are representative of the set of 40 stations, and further confirms that the model overpredicts the St. Louis observations.

Other investigators who have included consideration of diurnal variations in emission rates in their analysis have generally obtained

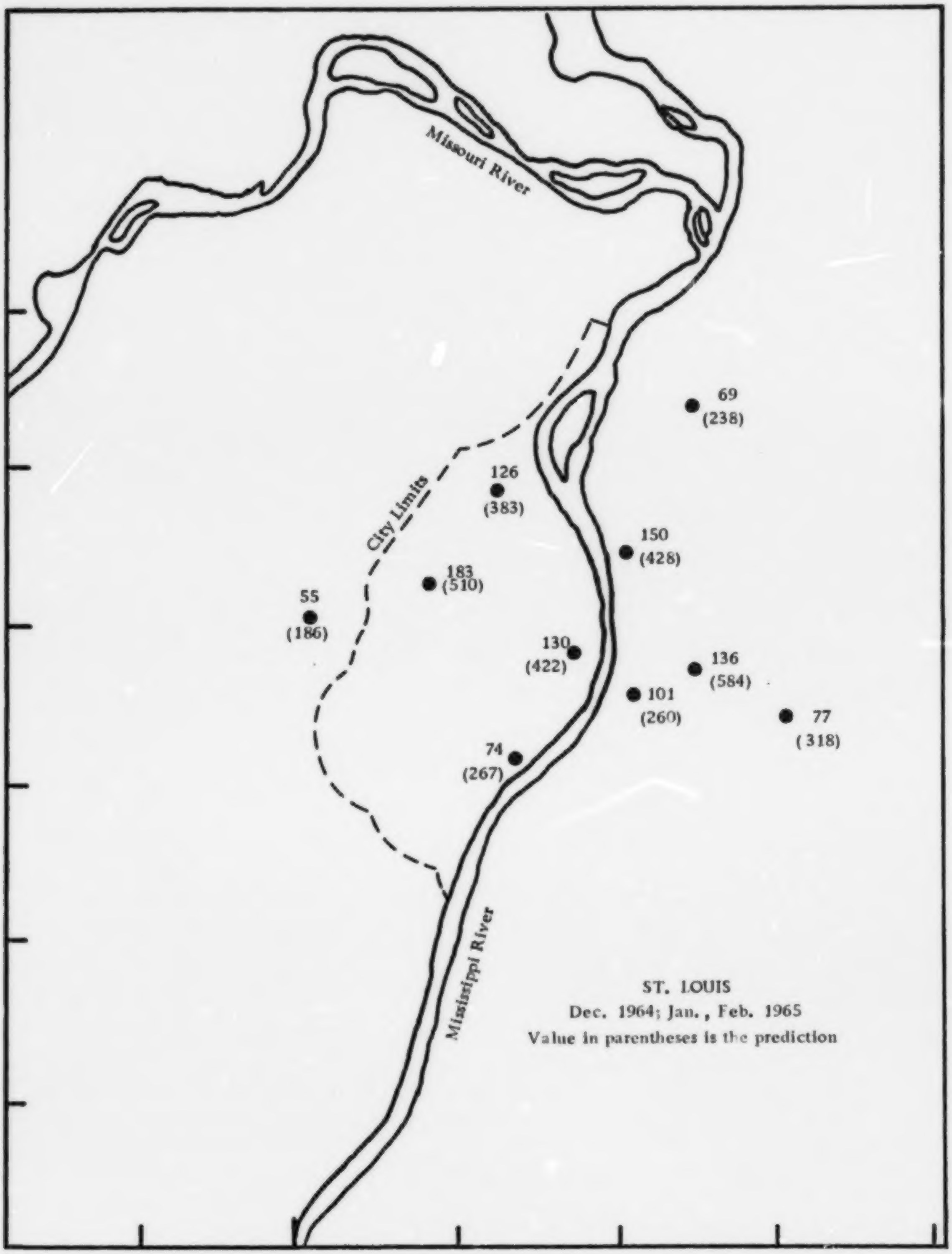

Missouri River
69
(238)
126
(383)
City Limits
150
(428)
183
(510)
55
(186)
130
(422)
136
(584)
101
(260)
77
(318)
74
(267)
Mississippi River
ST. LOUIS
Dec. 1964; Jan., Feb. 1965
Value in parentheses is the prediction

Figure 34. Seasonal Mean Observed and Predicted Concentrations (from Calder, 1970) Using Seasonal Mean Emission Rates

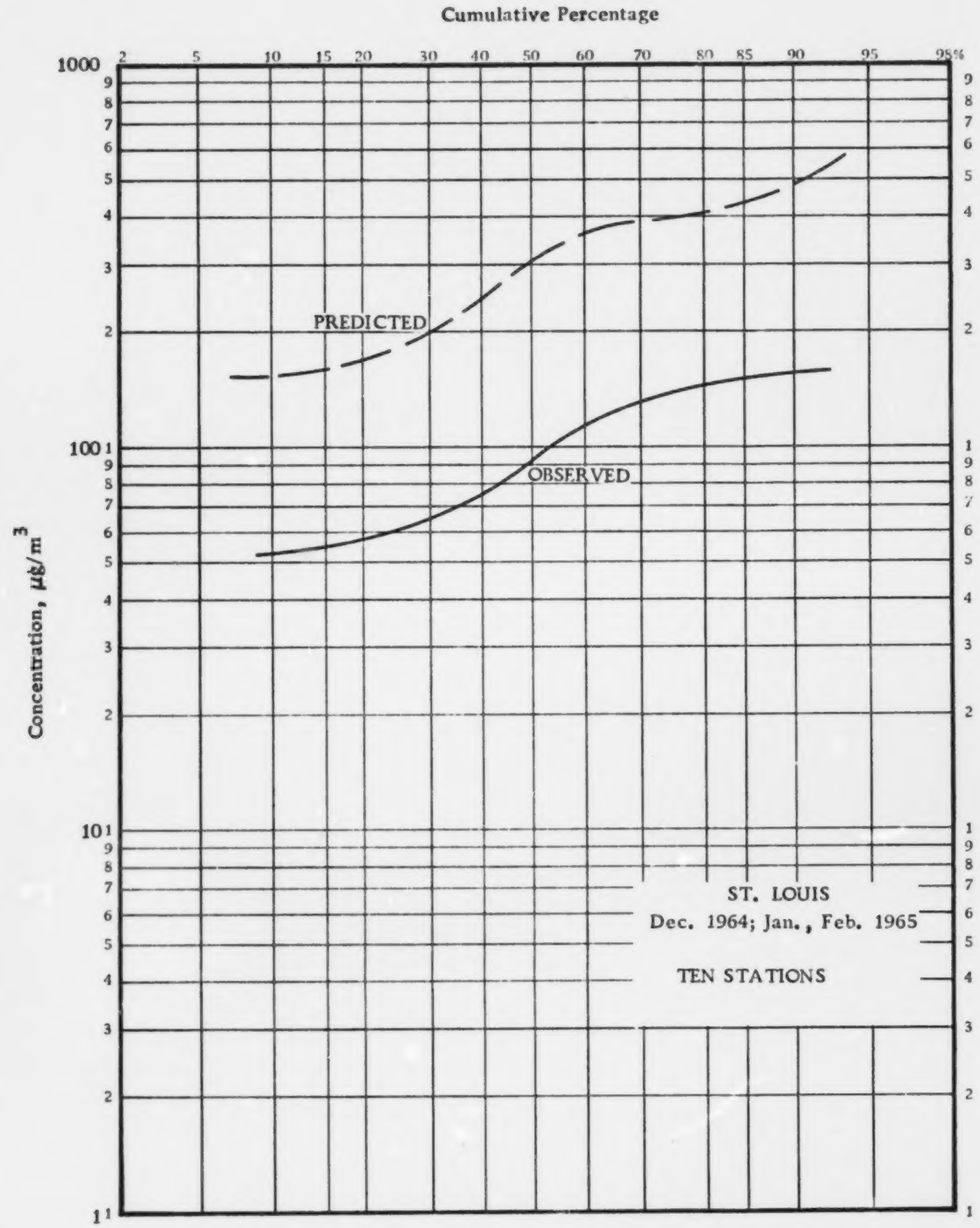


Figure 35. Frequency Distribution of Seasonal Mean Observed and Predicted Concentrations Using Seasonal Mean Emission Rates (Data from Calder, 1970)

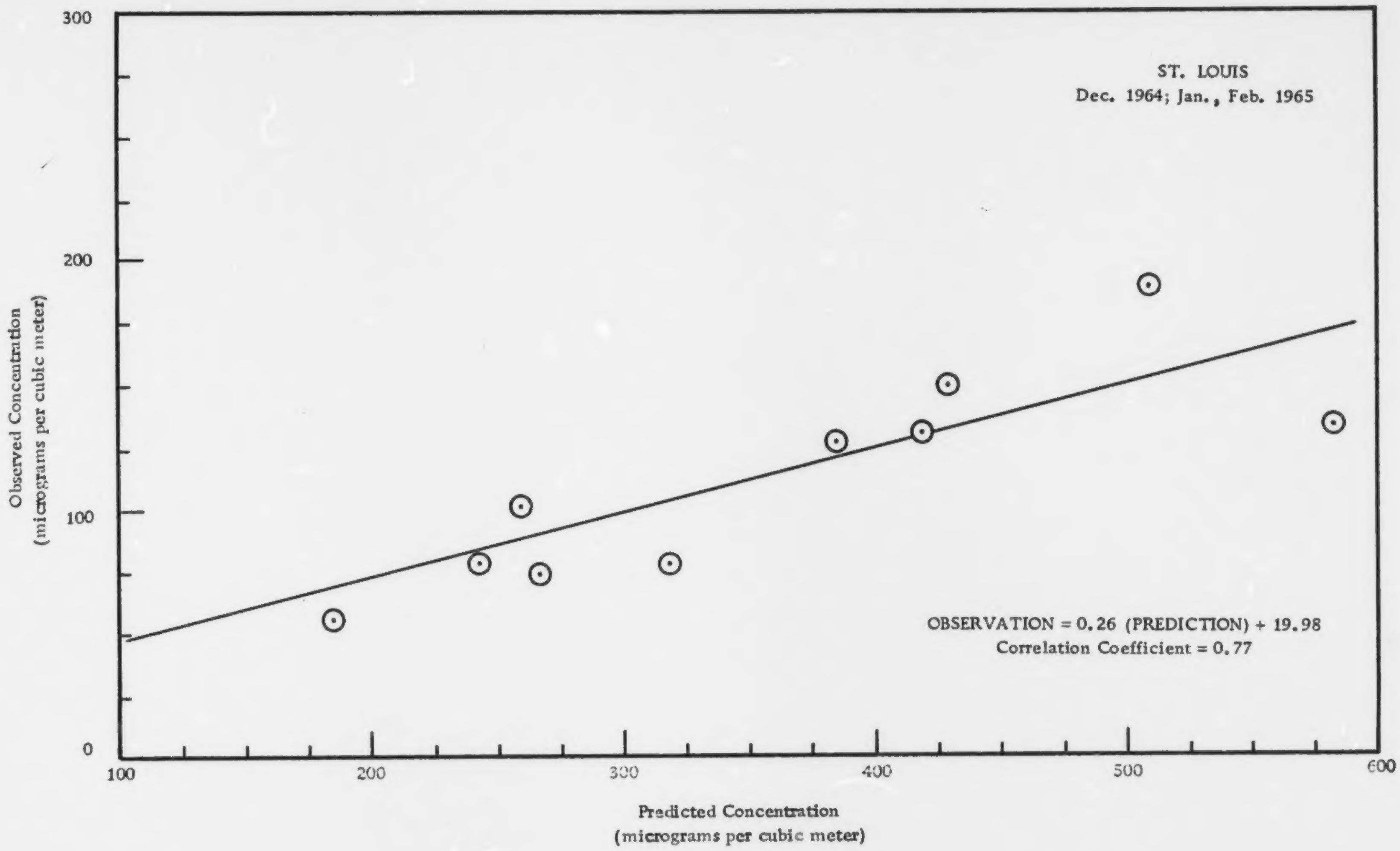


Figure 36. Regression of Observed Concentrations on Predicted Concentrations from Calder (1970)

better results. For example, Miller and Holzworth have computed the city-wide average concentration for selected early morning and afternoon two-hour periods in Nashville on 31 selected days. The frequency distributions of predicted and observed concentrations obtained from this analysis are shown in Figures 37 and 38. The Miller and Holzworth model is a rather extreme simplification of the Gaussian plume model for urban diffusion analysis which completely ignores spatial variations in emission rates by use of a city-wide average. Therefore, no resolution of the spatial distribution of concentrations is possible with this model. This model has been recommended as a method of estimating regional air quality where suitable monitoring observations are not available and no single source is the principal cause of pollution levels (Federal Register, 36, August 14, 1971, Part II).

Turner, who devised the scheme (based on the degree day concept) for estimating diurnal variations in SO_2 emission rates in the Nashville data used by Miller and Holzworth, used a more extensive set of the same data to compute 24-hour average concentrations which included consideration of the diurnal variation in emission rates (Turner 1964). His results are not reported in enough detail to construct frequency distributions; however, he reports that 43.7 percent of his predicted two-hour concentrations at seven stations were within ± 0.01 ppm (about 27 mg/m^3) of the observed concentration. For 24-hour observations at the same seven stations he found that 58.1 percent of predicted values were within ± 0.01 ppm.

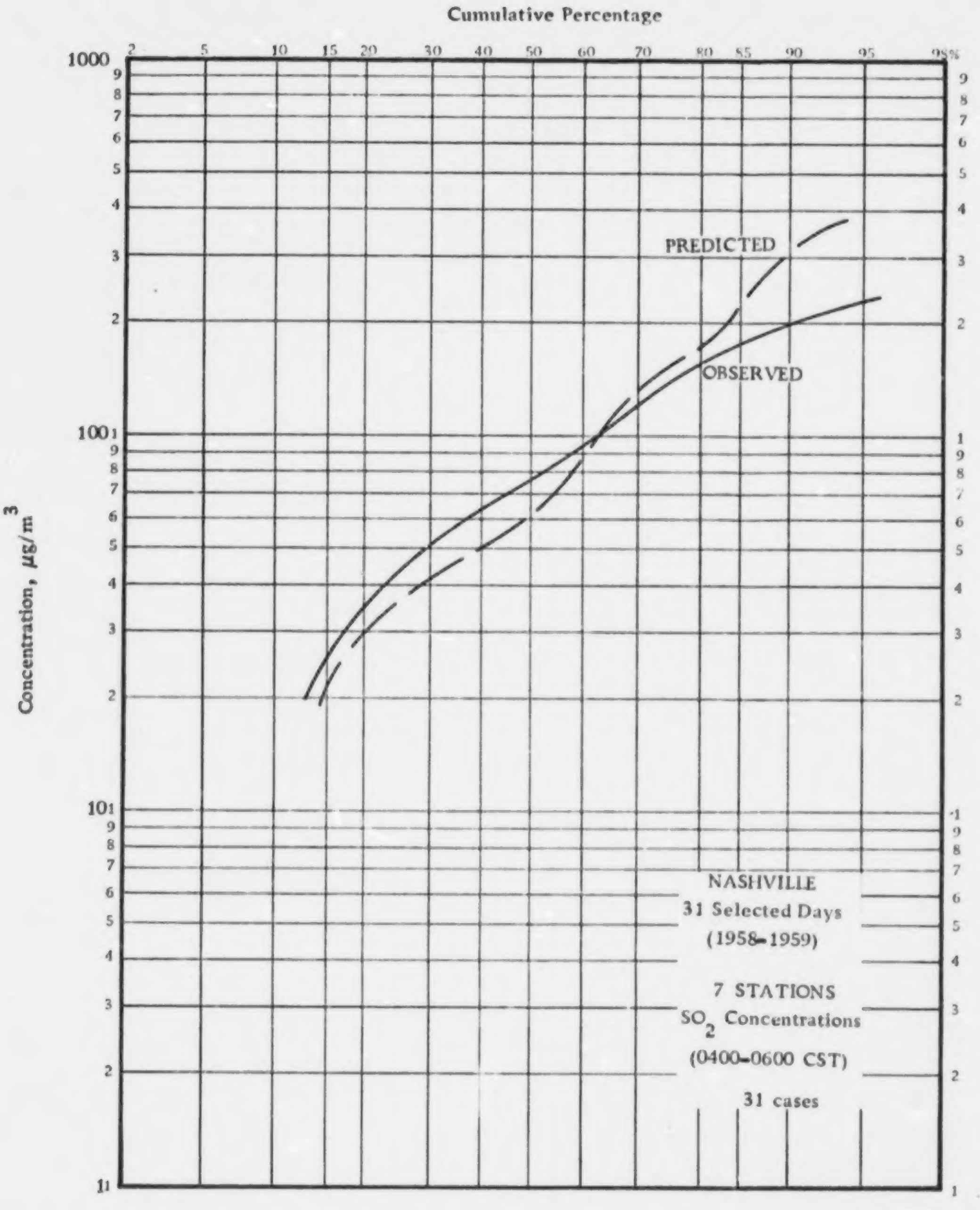


Figure 37. Observed and Predicted Frequency Distributions of Early Morning Concentrations Reported by Miller and Holzworth (1967)

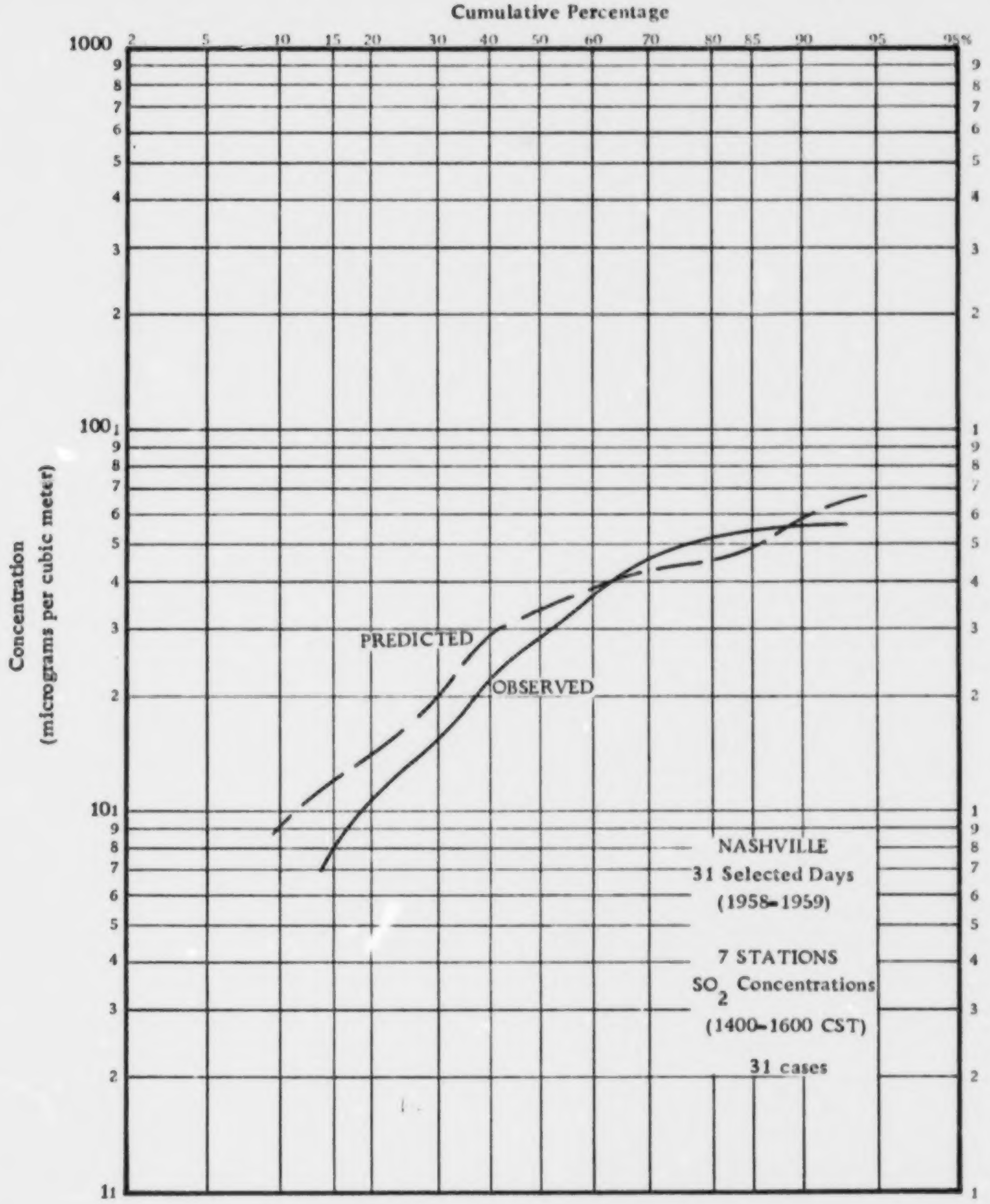


Figure 38. Observed and Predicted Frequency Distributions of Afternoon Concentrations Reported by Miller and Holzworth (1967)

More recently, Fortak (1969) reported results with a Gaussian plume type of urban diffusion model. The frequency distribution of predicted and observed hourly SO_2 concentrations at Sites #1 and #4 in Bremen, Germany, for the 1967-68 heating season are shown in Figures 39 and 40. Average daily emission rate estimates were determined by Fortak for these calculations. The graphs included represented the best and the worst agreement obtained by Fortak at four sites. He points out that Site #4 was in the vicinity of a large plant, and he attributes the observed high concentrations to uncontrollable, and unaccounted for, low-level emissions from the nearby plant. At Site #1 the agreement between the distribution of predicted and observed concentrations is almost as close as that obtained in this study for the St. Louis data.

The results cited above, and those from this study, show that the use of temporal variations in SO_2 in emission rates in concentration calculations leads to a realistic determination of the frequency distribution of short-term concentrations over a seasonal period, as well as a more accurate estimate of the seasonal mean concentration.

4.4 FINDINGS

A summary of the preceding results on the validity of the Gaussian plume type of multiple source urban diffusion model is given below. These results are based on the predicted and observed concentrations of SO_2 at 8 locations in Chicago during January 1967 and 10 stations in St. Louis during December 1964 to February 1965. The predictions used hourly estimates of meteorological and emission parameters. The atmospheric stability was estimated from hourly weather observations

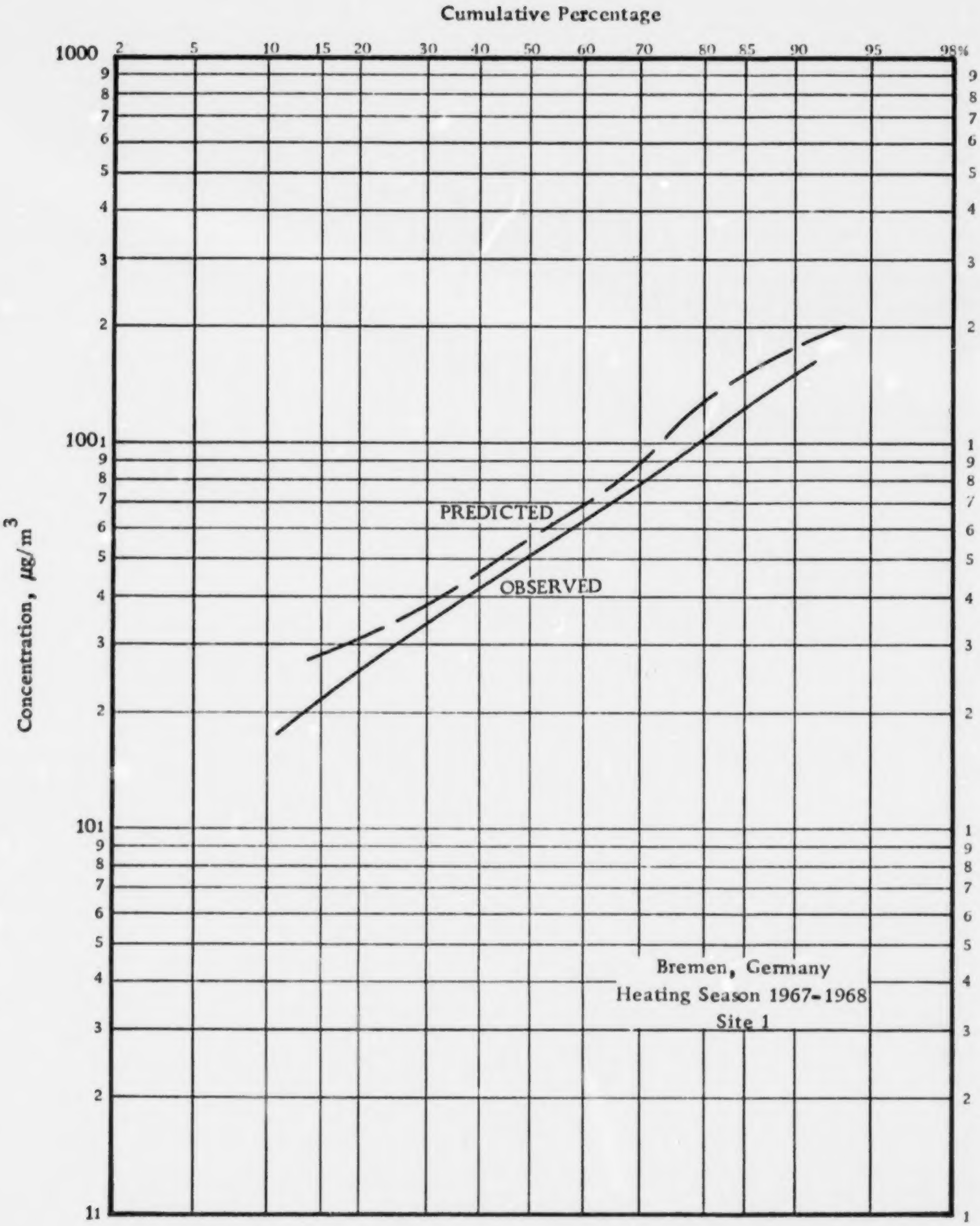


Figure 39. Observed and Predicted Distributions of Hourly Concentrations for Site 1 in Bremen, Germany, Reported by Fortak (1969)

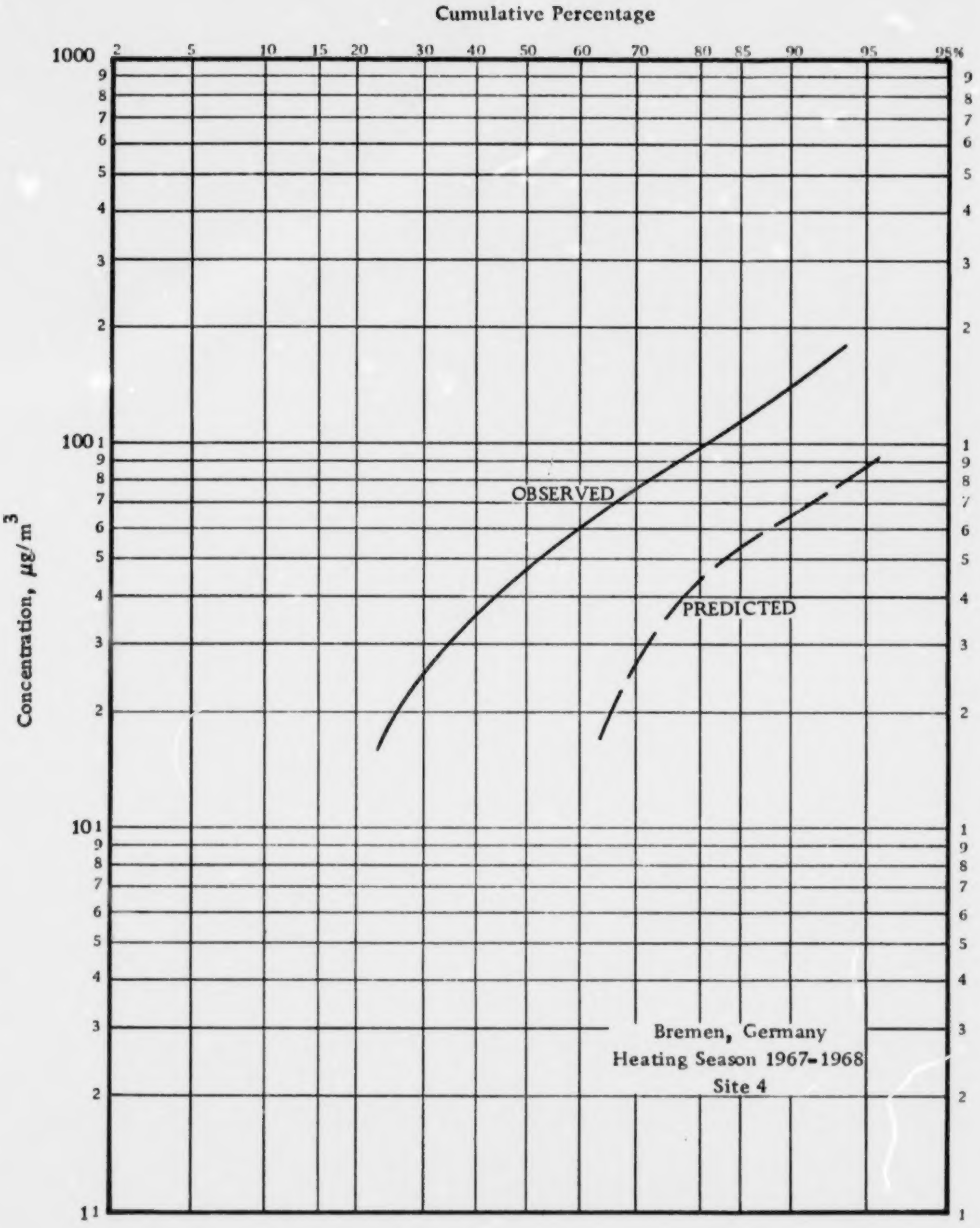


Figure 40. Observed and Predicted Frequency Distribution of Hourly Concentrations for Site 4 in Bremen, Germany, Reported by Fortak (1969)

from an adjacent airport using the McElroy-Pooler diffusion parameters based on Turner's definitions of stability categories. The mixing layer ceiling was estimated from radiosonde observations taken twice daily from remote locations (100 to 200 miles away). The wind speed and direction were hourly averages of several 3 in St. Louis, 8 in Chicago) continuous records. The emission rates of the largest sources were identified and located individually. For other sources a mean emission rate per unit area was estimated for a square gridwork of points with a one mile spacing between adjacent points. Each emission rate was related to hourly estimates of space heating and other operating requirements.

The findings are summarized as follows:

1. Predicted long-term (month or season) concentrations averaged over several locations are in good agreement with observed concentrations.

2. Predicted long-term concentrations at individual locations show a root-mean-square-error equal to about half the mean and indicate a slight tendency to overestimate more often than underestimate observed concentrations.

3. Predicted short-term (one or two hours) concentrations at individual stations show larger deviations from observed concentrations than do the long-term predictions. However, over a period of a month, or a season, the overall distribution of predicted short-term concentrations closely approximates the distribution of observed concentrations.

4. Proportionate stratified sampling is an effective method of selecting a limited set of short-term periods which adequately define a representative distribution of short-term concentrations in a long-term period. One hour out of 24 is a sufficient sample size for a three month period if the selected hour is varied to include all hours of the day.

5. The calm, or light wind, case is not adequately treated by the Gaussian plume type of urban diffusion model. Further study of procedures for applying the model to this type of situation is needed.

Section 5.0

SENSITIVITY ANALYSIS

Sensitivity is formally defined as the partial derivative of a model's output with respect to its input. In the case of complex models, however, a more practical definition, which is often employed for analytical purposes, is the incremental change in output resulting from an incremental change in input.

In a numerical simulation model as complex as the one utilized in this report, it is not possible to study all aspects of sensitivity analytically, nor is it safe to infer sensitivities from the form of the Gaussian model, which is the kernel of the simulation, because of the numerous interactions involved. Proper analyses require appropriate numerical exercising of the complete simulation.

Sensitivity analyses of urban pollution models have been reported by Hilst (1970) and Milford, et al. (1970a; 1970b). Hilst applied sensitivity analysis concepts in an example case study of the TRC Region Model, developed for the State of Connecticut, which involved a combination of a trajectory-oriented Gaussian model with the puff version for area sources and the plume version for major point sources. Hilst's results are of interest, but as he attests, limited in scope by the case study nature of the analysis.

The work reported by Milford, et al., deals with the variations of the model developed for the New York/New Jersey/Connecticut Air Quality Region. The studies which they have reported describe a model which bears a general resemblance to the steady-state plume model implemented in the study covered in this report. Their work, however, is very specifically oriented in form, input, and application to the greater New York area, and their reported sensitivity results focus largely on highly specific individual case examples, rendering useful generalizations difficult. The study in this report attempts to derive broad-scale significant sensitivity findings from a generally applicable model.

This section describes the work performed to analyze the sensitivity of the output concentrations of the multiple-source Gaussian plume diffusion model to model input parameters. Important questions to be answered by the analysis, which concentrates on the sensitivity of the short-term version of the model, with reference to the longer term climatological version where appropriate, are presented. The parameters and their value ranges are discussed, the methodology is described, and the analysis and results are presented. In the discussion of this section, the broad-scale significant findings, where sensitivity exists, are presented in summarized form. Appendix F contains descriptions and samples of the computer printouts which give complete listings of the sensitivity computations.

5.1 ELEMENTS INVESTIGATED

The principal points which the sensitivity analysis addresses are presented in question format as follows. The analysis was approached from this point of view in order to focus on questions which are considered to be of the greatest practical significance, and the results are intended to be definitive with regard to these questions. The questions are identified in terms of type of model input, and each is subsequently discussed in greater detail in the cited sections.

1. Spatial Variability of Emission Rates. The question here concerns the scale of variability in area source emission rates which can impact significantly on model predictions. The two considerations of primary interest in this question are the fineness of the grid used to represent area sources, and the basis used for separating significant point sources from area sources (Section 5.4.1).

2. Vertical Distribution of Area Source Emissions. This question concerns the extent to which various vertical distributions in the assumed emission height, and buoyancy rise, of area source emissions may affect model predictions (Section 5.4.2).

3. Vertical Diffusion Parameters. This question addresses the extent to which variations in the power law functions, which are used to represent the vertical spread of pollutants with travel distance, affect the model outputs (Section 5.4.3).

4. Decay Rate. The question here concerns definition of the conditions under which this parameter significantly affects outputs (Section 5.4.4).

5. Wind Speed and Wind Profile Power Law. The question of model sensitivity to wind speed is normally straightforward, and becomes complicated only when a decay rate exists. For zero decay, the model sensitivity to wind speed is only slightly complicated by interaction with the wind profile power law. Thus, the question of model sensitivity

to both wind speed and the vertical wind speed profile power law is examined (Section 5.4.5).

6. Mixing Ceiling. This question concerns the significance of uncertainties in this parameter (Section 5.4.6).

7. Wind Direction. The question here concerns the degree of resolution in wind direction to which the model output is sensitive (Section 5.4.7).

8. Diurnal Variation in Emission Rate. The main question here concerns the effect, on the predicted long-term average concentrations, of any correlation of diurnal variations in emission rates with diurnal variations in meteorological conditions (Section 5.4.8).

5.2 PARAMETER RANGES AND COMBINATIONS

Each of the sensitivity points raised in Section 5.1 focuses on the sensitivity of the model to certain specific model inputs, and all of the model inputs are incorporated in one or more of these questions. In order to design model sensitivity experiments, it is necessary to define a reasonable range of interest for each model input and to select combinations of values of all input parameters to use in testing for sensitivity. It will be seen that the inputs can be represented by a small number of values scattered over the total range of values of interest.

Sensitivity analysis in this program is focussed on changes in calculated concentrations which are associated with changes in input for a given set of input values. In view of the large number of such comparisons which are possible in the context of the preceding eight questions, the first step is to define reasonable ranges of interest for each parameter; subsequently, determination was made of which parameters have little influence on output over their defined range of values, and the remaining parameters were analyzed in more detail.

The initial set of parameters and the specific input values selected for use in the sensitivity analysis are shown in Table 25. The values selected were based on the judgement and experience of the in-house staff of diffusion meteorologists, as well as, to some extent, on the numerical information developed in the course of the validation study (Section 4.0). The following comments on the values selected for certain of the parameters are in order at this point:

- Decay Half-Life: One obvious choice is for no decay (infinite half-life); the other (30 minute half-life) represents a moderately reactive material. (A third extremely short half-life (5 minutes) was experimented with to a small degree, with results reflected in Section 5.4.3.)
- Wind Speed: The three values are intended to reflect light, moderate and strong anemometer-level winds.
- Wind Profile Power: Two values, arbitrarily chosen as depicting the range.
- Wind Direction: (See Sections 5.4.1 and 5.4.7.)
- Mixing Ceiling: A very low value, an intermediate (characteristic) value, and a high value.
- Diffusion Function and Stability Class: The three cases represent extreme atmospheric stability, neutral stability, and extreme instability.

Table 25. Sensitivity Parameters, Ranges and Selected Values

Parameters	Units	Range	Selected Values
METEOROLOGICAL AND POLLUTANT:			
Pollutant Half-Life*	min	0-∞	30;∞
Wind Speed	m/sec	1-20	2, 6, 18
Wind Profile Power	--	0.1-0.5	0.15, 0.3
Wind Direction	azimuth deg.	0-360	--
Mixing Ceiling	m	100-∞	100; 500; 2500
Diffusion Function and Stability Class	m	--	Pasquill Class E McElroy-Pooler Class D McElroy-Pooler Class 1
EMISSION AND RECEPTOR:			
Number of Point Sources	--	--	(1) All major sources (51 for St. Louis) (2) All with Annual Emissions within 10% of Largest Emitter (19 for St. Louis) (3) None (all aggregated into area sources)
Area Source Grid Spacing	miles	--	(1) 0.25 (2) 1 (3) 4
Distribution of Emission Heights for Area Sources	--	--	(1) All at Mean Height (2) 50% at Mean Height, 25% at 1/2 Mean Height and 25% at 3/2 Mean Height
Treatment of Diurnal Variations in Emissions	--	--	(See Section 5.4.8)
Receptor Location with Respect to Source Area	--	--	(1) Upwind Zone (2) Central High Emission Zone (3) Downwind Zone

*An "infinite" half-life represents a material that is essentially stable, or non-reactive, in the atmosphere, and corresponds to a zero decay rate. A 30-minute half-life is equivalent to a decay rate of 0.0231/min.

- Number of Point Sources: See discussion in Section 5.4.1.

- Area Source Grid Spacing: See discussion in Section 5.4.1.

- Distribution of Emission Heights for Area Sources: See discussion in Section 5.4.2.

- Treatment of Diurnal Variation in Emissions: See discussion in Section 5.4.8.

- Receptor Location with Respect to Source Area: See discussion in Sections 5.4.1 and 5.4.7.

In addition to the parameters listed in Table 25, there is a need to define a selection of basic geographic patterns of emission rates, as well as the selection of receptor locations relative to this pattern at which to measure sensitivity effects. It seems reasonable to define three principal, general situations concerning the relationship of a receptor relative to an emission pattern:

1. The receptor is in an area of relatively uniform emissions with no significantly strong upwind sources (upwind receptor).

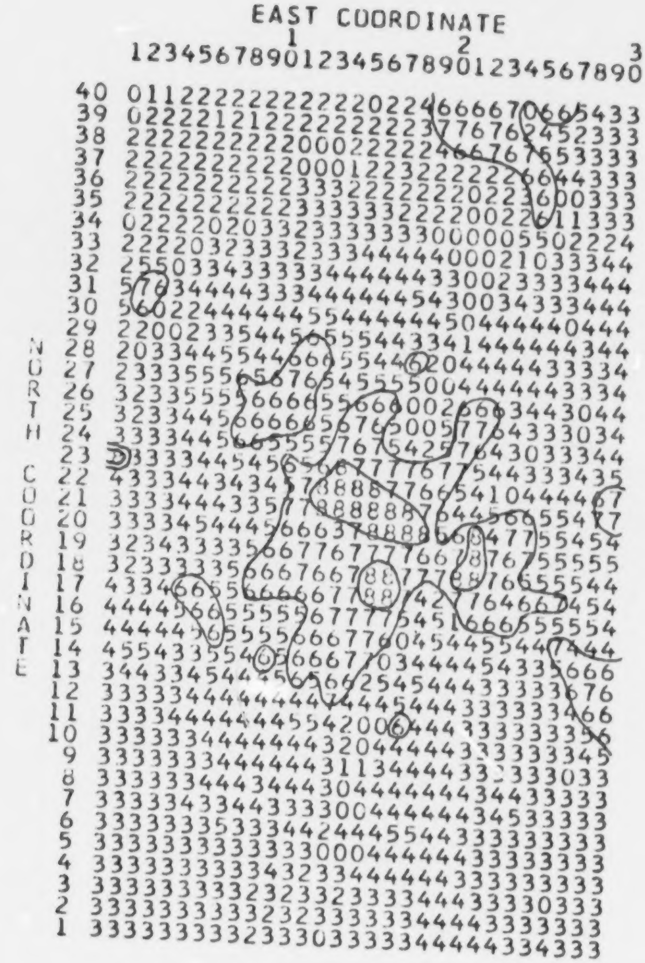
2. The receptor is in an area of high emission rates surrounded by noticeably lower upwind emission rates (as in the center of urban area), (center receptor).

3. The receptor is in area of light or moderate emissions with significant upwind sources (downwind of urban center), downwind receptor).

In the validation analysis the relative contribution to the total emissions arising from point sources in contrast to area sources had already been defined for the receptor locations which represent sampling stations. From these results it was noted that, in by far the majority of the cases examined, the overall contribution from point sources was small. There were notable exceptions in which the point sources were the dominant contributors to particular receptor locations under particular conditions. The impact of such special situations is examined further in Section 5.4.7. Meanwhile it was determined that the first order of importance was to examine realistic patterns of area source emissions, in order to assist in the definition of emission rate patterns and the associated receptor locations for use in the sensitivity analysis.

The area source emission rates for each square mile and each hour in the 2036-hour St. Louis data sample had been previously stored on magnetic tape for use in the validation analysis. These data were retrieved and used to generate hourly contour maps of the area source emission rates, which were then studied to determine whether consistent patterns were present. Three sample maps are shown in Figures 41 through 43. These represent relatively extreme variations in emission patterns over the 89-day period. These figures illustrate the general observation that, although the magnitude of emissions at any point may vary by a factor of as much as ten, the distribution of the pattern remains relatively consistent. No outstanding variation in the general shape of the pattern was noted with time of day or day of week. As a result, it was decided that the three receptor location characteristics described above (upwind, center and downwind) could be reasonably represented by a single emission pattern with three such receptor locations. The selected pattern is that shown in Figure 42. The wind

SYMBOL	RATE, G/SEC	SYMBOL	RATE, G/SEC
0	0.0 TO 0.01	5	1.00+ TO 3.00
1	0.01+ TO 0.03	6	3.00+ TO 10.00
2	0.03+ TO 0.10	7	10.00+ TO 30.00
3	0.10+ TO 0.30	8	30.00+ TO 100.00
4	0.30+ TO 1.00	9	OVER 100.00



```
                 EAST COORDINATE
                    1         2         3
           123456789012345678901234567890

       40  011222222222220224666670665433
       39  022221212222222223776762452333
       38  222222222200022222466767653333
       37  222222222200012232222226644333
       36  222222222233322222220223600333
       35  222222222233333322220022611333
       34  022220203323333333000005502224
       33  222203233323334444400021033344
       32  255033433333444444330023333444
       31  576344443334444445430034333444
       30  560224444445544444450444440444
       29  220023354455555443341444444344
       28  203344554466655446204444433334
       27  233355565676545555004444443334
       26  323355556666556660026663443044
       25  323344566666567650057764333034
       24  333344566555576754257643033344
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       17  433466556666677887742764667454
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       15  444445655556667760454455447444
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       12  333334444444444444544433333676
       11  333344444445542006444333333466
       10  333333444444443204444433333356
        9  333333344444431134444433333345
        8  333333444344430444444443333033
        7  333334334443333004444443443333
        6  333333353334424445544345333333
        5  333333333333300044444433333333
        4  333333333343233444444433333333
        3  333333333232332333344443333333
        2  333333333323233333334443330333
        1  333333332333033333344444334333
```
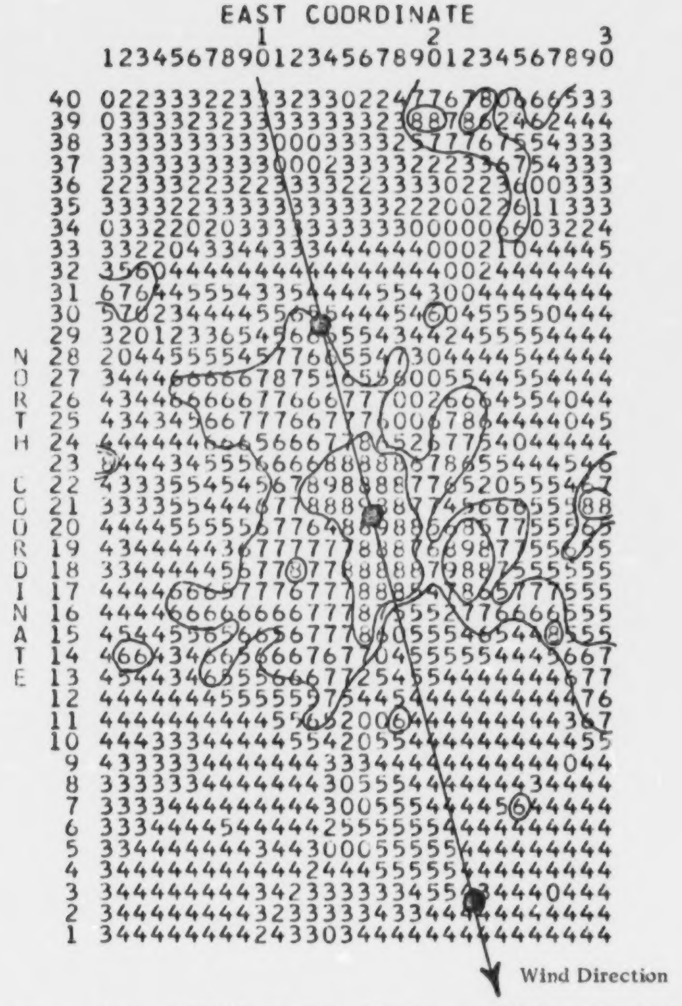

FIGURE 41. ST. LOUIS AREA SOURCE EMISSION RATES, 1AM DECEMBER 2, 1964.

● Receptor Location

SYMBOL	RATE, G/SEC	SYMBOL	RATE, G/SEC
0	0.0 TO 0.01	5	1.00+ TO 3.00
1	0.01+ TO 0.03	6	3.00+ TO 10.00
2	0.03+ TO 0.10	7	10.00+ TO 30.00
3	0.10+ TO 0.30	8	30.00+ TO 100.00
4	0.30+ TO 1.00	9	OVER 100.00



```
                  EAST COORDINATE
                           1         2         3
                  123456789012345678901234567890

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              39  033332323333333323887862462444
              38  333333333300033332577767554333
              37  333333333300023333222336754333
              36  223332232223332233330223600333
              35  333322333333333332220022611333
              34  033220203333333333000006603224
              33  332204334433344444400021044445
              32  356044444444444444400244444444
              31  676445554335444455430044444444
              30  570234444556854445460455550444
              29  320123365456655434424555554444
           N  28  204455554577665547304444544444
           O  27  344466666678755655005544554444
           R  26  434466666776667770026664554044
           T  25  434345667776677760067864444045
           H  24  444444666566677865267754044444
              23  444434555666688888678655444546
           C  22  433355454567898888776520555467
           O  21  333355444677888988774566655588
           O  20  444455555677648898866867755565
           R  19  434444436777777888768987755655
           D  18  334444445677877888887988755555
           I  17  444466657776777888547865777555
           N  16  444466666666777875552776666555
           A  15  454455656656777860555465448555
           T  14  466434665666767704555554445667
           E  13  454434655566667725455444444677
              12  444444455555975444544444444476
              11  444444444445565200644444444367
              10  444333444444554205544444444455
               9  433333444444433344444444444044
               8  333333444444430555444444434444
               7  333344444444430055544445644444
               6  333444454444425555554444444444
               5  334444444344300055555444444444
               4  344444444444424445555544444444
               3  344444444342333333455634440444
               2  344444444323333343344444444444
               1  344444444243303444444444444444
```
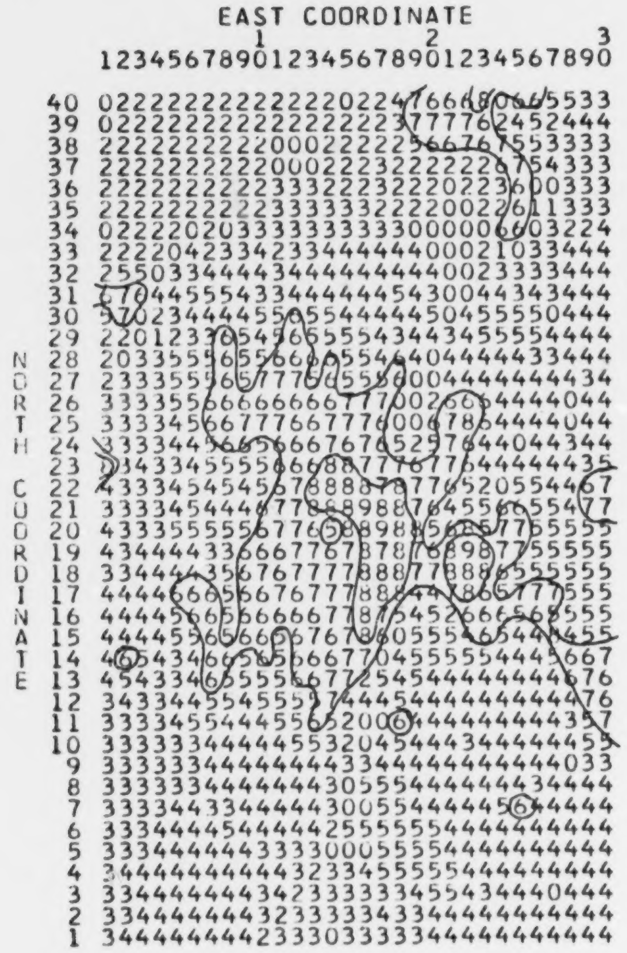

FIGURE 42. ST. LOUIS AREA SOURCE EMISSION RATES,
1PM DECEMBER 5, 1964.

SYMBOL	RATE, G/SEC	SYMBOL	RATE, G/SEC
0	0.0 TO 0.01	5	1.00+ TO 3.00
1	0.01+ TO 0.03	6	3.00+ TO 10.00
2	0.03+ TO 0.10	7	10.00+ TO 30.00
3	0.10+ TO 0.30	8	30.00+ TO 100.00
4	0.30+ TO 1.00	9	OVER 100.00



```
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                        1         2         3
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          39   022222222222222223777762452444
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          36   222222222233322232220223600333
          35   222222222233333322220022611333
          34   022220203333333333000006603224
          33   222204233423344444400021033444
          32   255033444434444444440023333444
          31   670445554334444445430044343444
          30   570234444556554444450455550444
          29   220123365456655543443455554444
        N 28   203355565566665544404444433444
        O 27   233355565777665556004444444434
        R 26   333355666666667770026664444044
        T 25   333345667776677760067864444044
        H 24   333344566566676765297644044344
          23   334334555566688777767764444435
        C 22   433345454567888878776520554467
        O 21   333345444677868988764556655477
        O 20   433355555677658898856657755555
        R 19   434444336667767878768987755555
        D 18   334444356767777788877888655555
        I 17   444466656676777884478665777555
        N 16   444456656666667787545266656555
        A 15   444455656666767860555465444455
        T 14   465434665656667704555554445667
        E 13   454334655555667725454444444676
          12   343344554555574445444444444476
          11   333345544455652006444444444357
          10   333333444445532045444344444455
           9   333333444444443344444444444033
           8   333333444444430555444444434444
           7   333344334444430055444445644444
           6   333444454444425555554444444444
           5   333444444333300055554444444444
           4   344444444443233455555444444444
           3   334444444342333334555434440444
           2   334444444323333343344444444444
           1   344444444233303333344444444444
```

FIGURE 43. ST. LOUIS AREA SOURCE EMISSION RATES, 7AM DECEMBER 3, 1964.

direction was defined to be as shown (changes in direction are examined in Section 5.4.7), and the three solid circles were selected as receptor locations representing upwind, center (high emission), and downwind receptor zones.

The sensitivity analysis was therefore performed in the context of this representative background pattern of emissions, and the parameters listed in Table 25 were varied against this background.

5.3 METHODOLOGY

The methodology followed is a straightforward manipulative one, in which changes in input are used to define changes in output. The output changes are then examined as relative or absolute changes and ranked to determine those which are most significant. Short-term concentrations are emphasized in the analysis, and the sensitivity of long-term concentrations is addressed in the text as appropriate. The first step in the analysis consisted of computer runs representing a full factorial replication of all combinations of the inputs identified in Table 25 which are relevant to short-term concentrations. This includes all but wind direction and the magnitude of diurnal variations in emissions. The total number of combinations is 5832 (i.e., 2 pollutant half-lives x3 wind speeds x2 wind profile powers x3 mixing ceilings x3 diffusion functions x3 sets of point sources x3 area source grid spacings x2 sets of emission heights for area sources x3 receptor locations). Within this total, for each model input, two to three thousand sets of variations (depending on the input parameter involved) in model output were therefore generated for each specified variation in input.

Inputs which show little output variation over all sets, or almost all sets, were accordingly identified as insensitive inputs, and variation in these insensitive parameters was not considered further. Each of these is discussed in Section 5.4. The selection of a criterion which would represent a significant change in output over a range of input values was governed by the validation findings. As a result of those findings, it was decided that input changes must generate at least a 50 percent change in output for the range of input values considered in order to qualify as a significantly sensitive input. Where significant change was found, the analysis was pursued in greater depth, as is described in Section 5.4.

5.4 SENSITIVITY ANALYSIS RESULTS

In the following discussion, the results of the analyses of the computer runs described in Section 5.3 are presented in detail. The analytical procedure for defining the impact of each input parameter consists of identifying "sensitive" changes in calculated concentrations resulting when an input parameter is varied. A "sensitive" change is defined to be a change in the input parameter which results in a greater than 50 percent change in the calculated concentration. Such cases are then subjected to more detailed analysis.

5.4.1 Spatical Variability of Emission Rates

Urban diffusion modelers usually identify only the most significant point sources, and obtain reasonably accurate estimates of emission rates for these sources. Emissions from other sources are treated as uniformly distributed over a segment of area, and estimates of the emission rate per unit area are made for such convenient squares or blocks of the urban area. A square mile is a frequently used block size.

The actual computational treatment employed in evaluating the effects of these selected block sizes on urban air pollutant concentrations may sometimes involve further assumptions regarding the distribution of source within each block (e.g., use of point sources, normal line source, virtual point source, or uniform area source concepts to represent each block mathematically.)

In this study the overall area source input data are represented by a gridwork of point locations, each with its own emission rate per unit area, and thus describing a smooth continuous surface (in the mathematical sense) of area source emission rates. In the program computations, linear interpolation between points is used to define the emission rate as a continuous function of position in evaluating the effects of area source emissions. For sensitivity analysis purposes variation in the fineness of the area source representation is accomplished by changing the spacing between grid points and the corresponding block size in the area source emission inventory. The two questions of concern here are, What is the real spatial variability in emission rates? and, How accurately should the real spatial variability be reflected in the model? Since the real spatial variability is not known, except as estimated for square mile blocks, this parameter has been hypothesized for testing sensitivity. The assumption has been made that when a unit square mile area is divided into 16 quarter-mile squares, the emission rate per unit area for each subdivision will be approximately normally distributed (in a statistical sense) about a mean value with a standard deviation equal to one-half the mean. In the sensitivity analysis, mean values for square mile areas were used with a random number generator to define emission rates appropriate to the smaller quarter-mile squares. Standard IBM computer routines for random number generation and inverse normal function evaluation were used.

The basic computer model defined in Section 3.0 and the selected set of SO_2 emission data drawn from the St. Louis data sample were used to test whether changing the grid resolution (1 mile) to a finer (0.25 mile) or a coarser (4 mile) mesh had a significant effect on the calculations.

As a further sensitivity test, the effect of various levels of aggregation of point source emission data into the general area source emission rate was examined. This was done by comparing calculations when all (51), some (19), or none of the major sources were merged. The point source emission rates associated with the selected area source emission pattern are listed in Table 26. In addition to the two extreme cases of merging none or all of the point sources, the effect of merging just those points, whose emission rates were less than 10 percent of the largest emission rate, was examined (i.e., merging all but the highest 19 emission rates). The location of the point sources relative to the three sensitivity receptor locations is shown in Figure 44. In order to examine the effect of large point sources on the center receptor location, the wind direction was shifted as indicated in Figure 44 to see what effect that would have on the sensitivity results.

Table 26. Ranked List of St. Louis Point Source Emission Rates for 1300 LST, December 5, 1964

Rank	Identification Number	SO_2 Emission Rate, g/sec	Rank	No.	Rate	Rank	No.	Rate
1	44	2680	21	35	188	41	10	19
2	48	1560	22	11	174	42	17	19
3	49	1310	23	27	163	43	16	18
4	47	1280	24	32	120	44	25	18
5	30	1050	25	26	115	45	5	17
6	51	752	26	1	92	46	18	15
7	43	706	24	20	91	47	13	11
8	50	604	28	14	77	48	28	11
9	45	601	29	33	77	49	7	9
10	36	591	30	24	68	50	15	4
11	37	586	31	23	61	51	38	0
12	46	568	32	19	49			
13	42	529	33	40	43			
14	8	488	34	29	40			
15	4	433	35	3	36			
16	31	384	36	39	35			
17	41	353	37	12	33			
18	22	305	38	21	33			
19	2	277	39	9	29			
20	6	191	40	34	22			

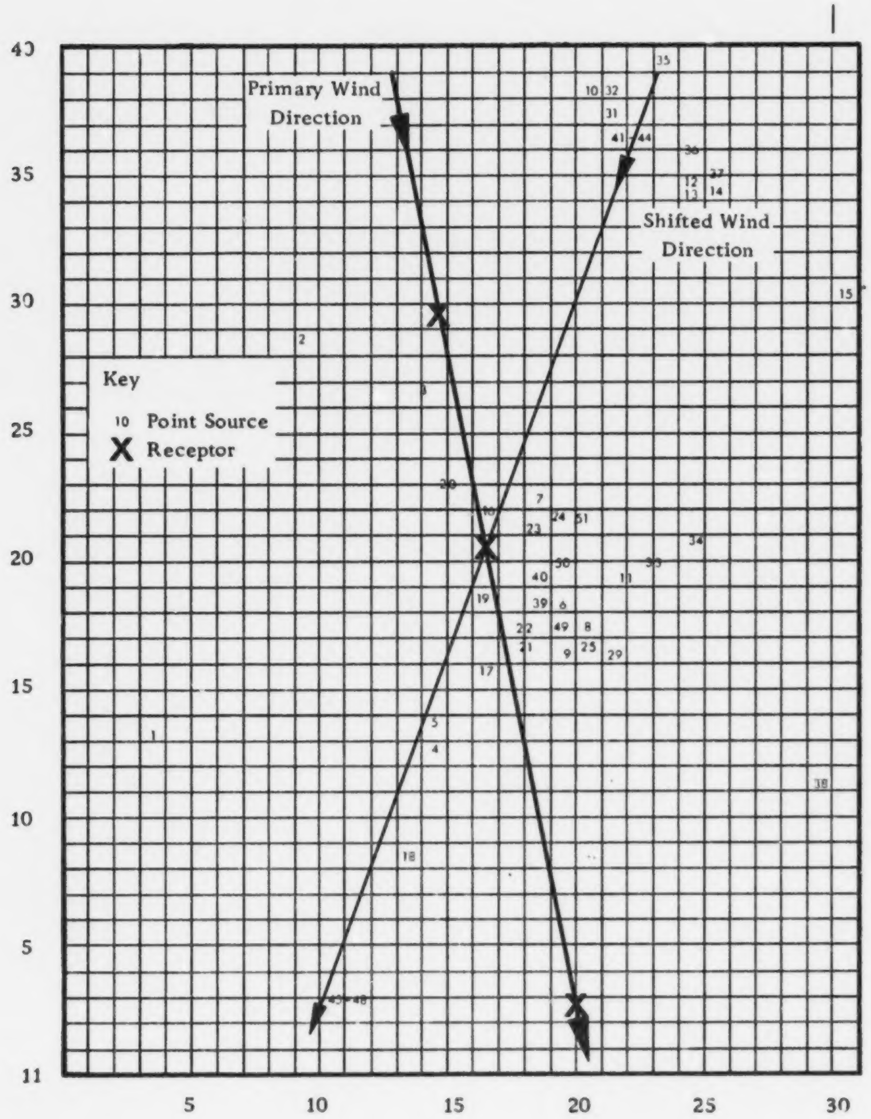
40
35
30
25
20
15
10
5
11
5
10
15
20
25
30
Primary Wind
Direction
Shifted Wind
Direction
Key
10 Point Source
X Receptor
35
10
32
31
41-44
36
37
12
13
14
15
2
3
20
7
16
24
51
23
34
30
33
40
11
19
39
6
22
49
8
21
9
25
29
17
5
4
1
38
18
45-48

Figure 44. Location of Point Sources in St. Louis Relative to Wind Directions and Receptor Locations in Sensitivity Analysis

Parenthetically, it will be seen in Section 5.4.2 and 5.4.5 that, when the initial large-scale screening analysis was performed, two parameters were immediately demonstrated to have only insignificant effects on the output concentrations. These two, the vertical distribution of area source emissions (5.4.3) and the profile power (5.4.5), were accordingly eliminated from the analysis in considering sensitivity to other inputs; at the same time, it was found possible to reduce the number of mixing ceilings considered (Section 5.4.6) from three (100, 500 and 2500m) to two (100 and 500m) for most of the detailed comparisons. Thus, the number of combinations considered in this section was reduced from 5832 to 972 (i.e., two pollutant half-lives x3 wind speeds x1 wind profile power x2 mixing ceilings x3 diffusion parameters x3 sets of point sources x3 area grid spacings x1 area source emission height x3 receptor locations). Of these, 324 represent the effect of a changing grid mesh size as a function of meteorological conditions in the presence of the standard of 51 individually identified point sources. When the 324 are examined in detail, almost half of the cases (141 cases or 47%) show significant changes in concentration (40% change) when the one- and four-mile spacings are compared. Similarly, 78 cases (24%) show show significant changes when the 1- and the 0.25-grid sizes were compared. When a shift in wind direction was considered, as shown in Figure 44, the number of sets yielding significant changes with a change in grid mesh size was reduced slightly.

These results show that averaging area source emission rates over areas larger than 1 square mile can lead to significant errors in estimated pollutant concentrations. Furthermore, if the standard deviation in emission rates of quarter mile squares (about 6 city blocks) is of the order of 50 percent of the mean over a square mile area, (as postulated in the beginning of this section), then even the use of square mile average emission rates can lead to significant errors in estimated pollutant concentrations.

Now, considering the impact of merging point sources into the area sources, we recall that this examination focuses primarily on the overall impact of such changes, rather than on the fine scale details of effects on specific receptors in the vicinity of significant point sources. The latter aspect is dealt with by Milford, et al. (1970a), and, because of its wind direction dependence, in Section 5.4.7 of this report. In the broader context, then, the following findings apply. For the smaller grid sizes (1 and 0.25 miles) only a negligible number (1-4%) of the cases show significant changes when the number of individual point sources is reduced from 51 to 19, and then to zero. For the coarse 4-mile grid, we find 4 percent of the cases showing significant concentration changes when the 19-source case is compared to the 51-source case, increasing to 18 percent when the "no-point-sources-considered" case is thus compared.

Therefore, we see that the broad-scale concentration picture is little affected either by treating individually, or by merging, various numbers of point sources when the area source grid scale is of the order of 1 mile or smaller; however, with a larger grid scale (of the order of 4 miles), failure to take into account at least the main point sources individually can cause problems. The 4-mile grid dimension was already questionable, of course, from the previously stated findings on grid size alone.

5.4.2 Vertical Distribution of Area Source Emissions

Area source emissions of SO_2 consist of a large variety of individual sources including stores, small plants, apartment buildings and small single and multi-family homes, to mention a few of the more common types. Since the emissions from these sources are primarily contained in burned fuel exhaust, the emissions are hot. As a result, the emissions are released from a variety of heights with a variety of plume rise effects. Although it is convenient to treat all emissions from a particular area as emanating from the same height, it may be unrealistic to do so. Various devices may be employed to simulate the vertical distribution, such as the use of multiple area source heights or the assumption of a vertical dimension in the initial plume.

An initial vertical distribution of pollutants has been simulated in this study by using multiple emission heights, and allocating the pollutant emission rate among those selected heights. In the sensitivity analysis, the results obtained by allocating 25 percent of the area emission rate to a height of one-half the mean emission height, and 25 percent to one and one-half times the mean emission height (leaving 50% emitted at emission height), are compared with those when all emissions in an area are at the same height. In terms of the initial set of 5832 input combinations there were 2916 pairs of such comparisons. In none of these was the concentration resulting from one distribution 50 percent greater than from the other. In fact, only in the case of a combination of high decay rate, low wind speed, and stable diffusion parameters, did one exceed the other by more than 25 percent. In general, the difference between the vertical distributions was negligible. As a result, in additional calculations, all emissions in any given area source were treated as emanating from a single height.

5.4.3 Vertical Diffusion Parameters

One way of expressing a basic hypothesis (the narrow plume concept), which was found to be acceptable in the model implementation described in Section 3.0, is that the scale of variability in emission rates (i.e., crosswind distance between significant changes in emissions) is large relative to the scale of variability in plume concentrations (i.e., the diffusion parameter σ_y). Furthermore, as was seen in Section 5.4.1, the contribution of point sources relative to that from area sources is significant only a small percentage of the time in terms of the broad concentration picture. As a result, the crosswind diffusion parameter is of only minor interest in the model. The impact of atmospheric turbulence and stability is manifested primarily in the vertical diffusion description.

The critical effect of choice of diffusion parameters for a "one-class change" in stability for the basic plume equation (single point source) is illustrated in Figure 45. This figure shows normalized concentrations (xu/Q) along the plume axis, as a function of downwind distance, from a point source at a height of 20 meters. The concentration is shown for the four combinations of two mixing-layer ceiling heights, 100 meters and 1000 meters, and two sets of diffusion parameters. One set corresponds to stable conditions using the E class of the Pasquill

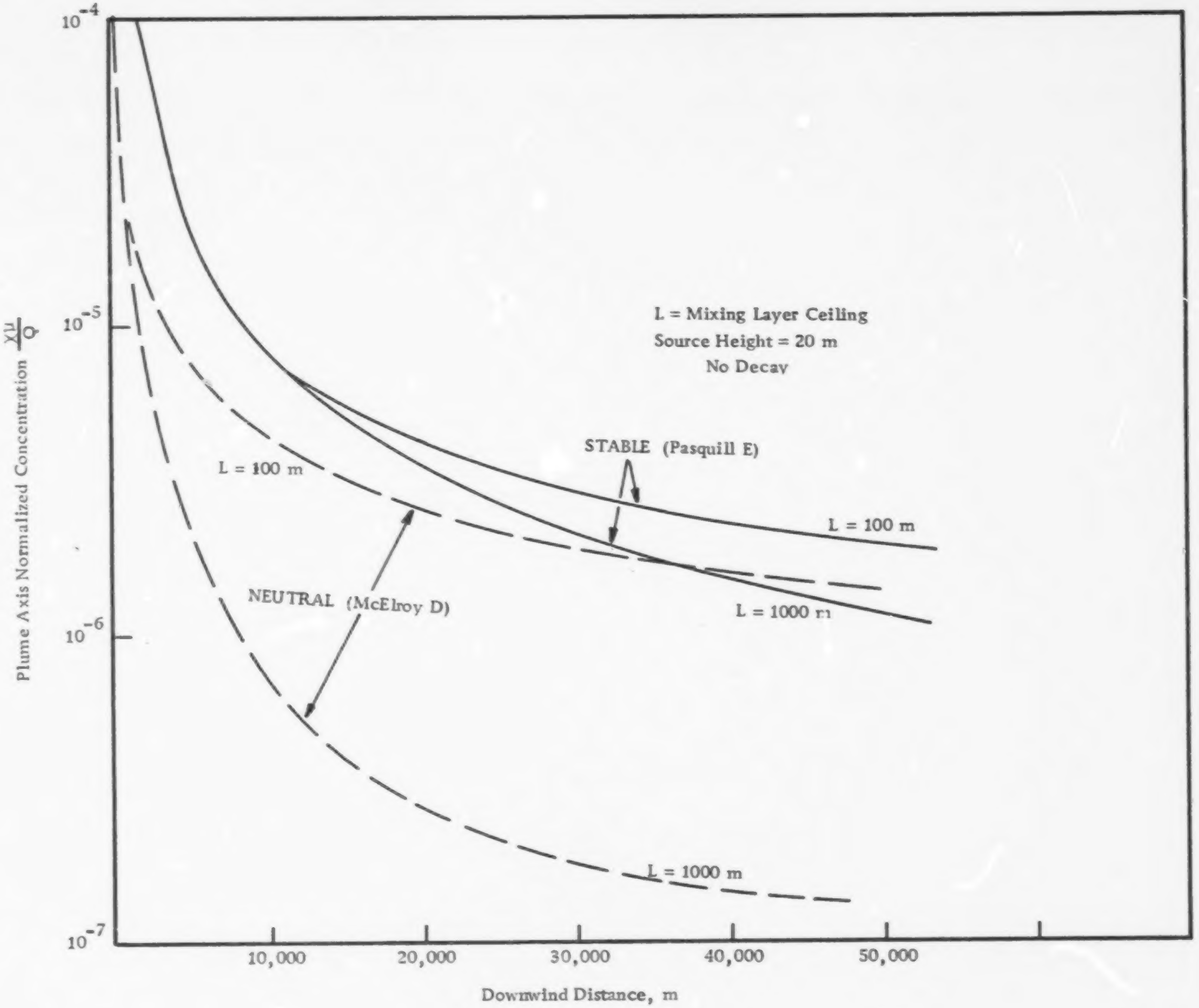

Figure 45. Example of Sensitivity of Normalized Concentration Field from a Point Source to Changes in Stability and Mixing Layer Ceiling

parameters; the other set corresponds to the McElroy-Pooler (1968) parameters based on the neutral Turner D stability category. The concentrations vary by a factor of 10 for the two sets of diffusion parameters when the mixing ceiling is only 100 meters and vertical diffusion is thus severely restricted.

From an analysis conducted separately from the general sensitivity study, the sensitivity of the model to the choice of a system of diffusion parameters is further illustrated in Figure 46. Model predictions for a three-week portion of the 89-day set of St. Louis data were made using first the McElroy-Pooler system of diffusion parameters based on the Turner stability classification system. The predictions were then repeated using the Pasquill system and Turner's stability criteria. The resulting frequency distributions of predicted 2-hour concentration are plotted along with the observed distribution. The distribution using the Pasquill-Turner system yields concentrations which are 40 to 70 percent higher than the McElroy-Pooler system for corresponding frequencies. This sensitivity examination is somewhat unusual in that it represents the effect of changing all stability inputs from one set to another.

A more detailed examination of the effect of variations in the vertical diffusion parameter (σ_z) is presented in Table 27. These values were selected from the extensive set of combinations of model inputs used in the general sensitivity analysis. They illustrate the complexity of the interrelationships of diffusion parameters with decay constant, wind speed and mixing ceiling. The most noticeable effect

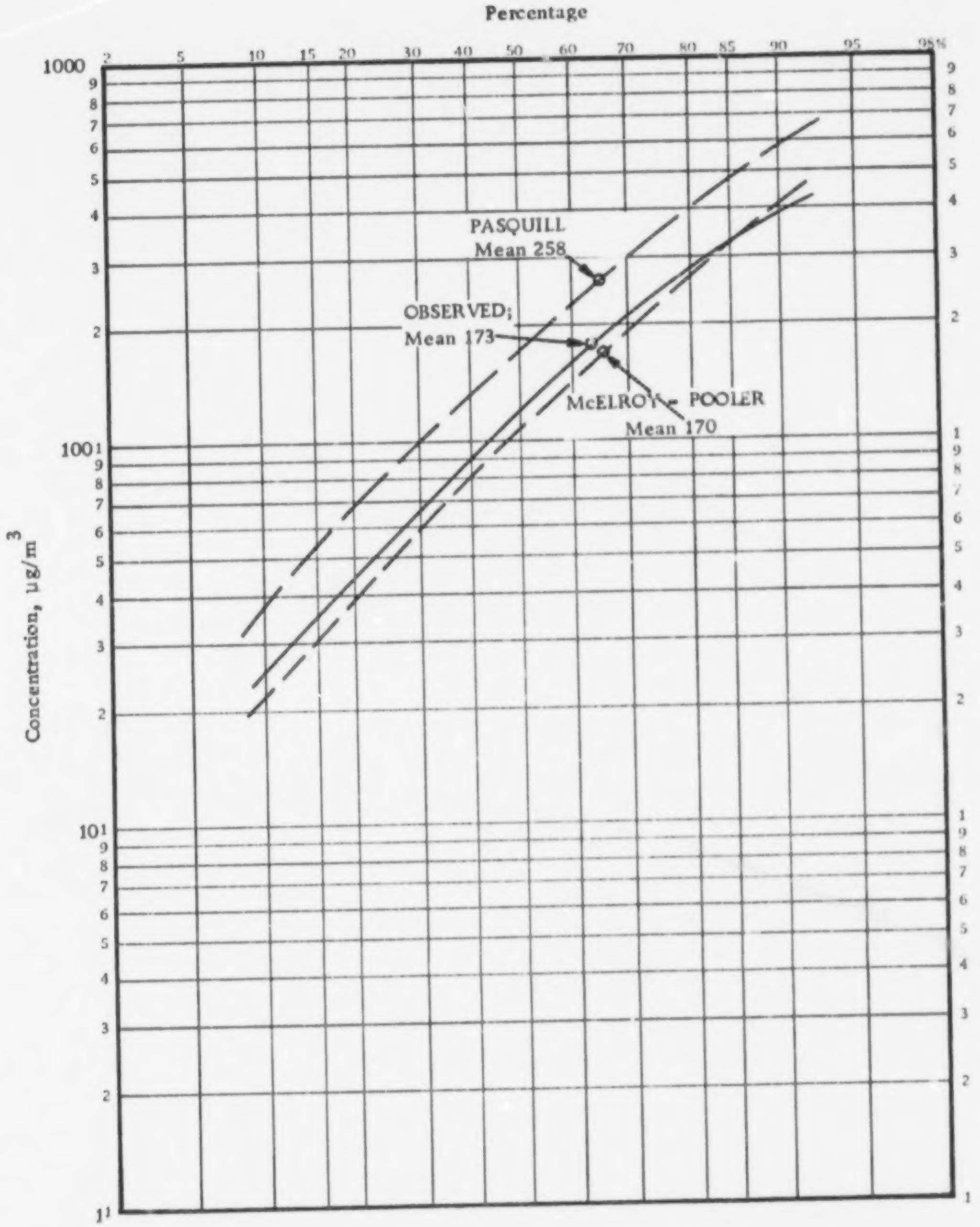

Figure 46. Comparison of Distributions of Two-Hour Model Predictions with Observations Using Two Different Systems for Assigning Diffusion Parameters and St. Louis Data Set for Ten Stations Combined

Table 27. Changes in Predicted Concentrations Resulting from Changes in the Vertical Diffusion Parameter

				Concentrations ($\mu g/m^3$) as a Function of Diffusion Parameters		
Receptor Location	Half-Life	Wind Speed, m/sec	Mixing Ceiling, m	Pasquill, Class E	McElroy-Pooler, Class D	McElroy-Pooler, Class 1
Center	No Decay	2	100	1259	1207	1274
Center	No Decay	6	100	547	402	425
Center	No Decay	18	100	182	134	142
Center	30 Min.	2	100	1146	819	850
Center	30 Min.	6	100	478	347	364
Center	30 Min.	18	100	174	127	134
Upwind	No Decay	2	500	12	3	2
Center	No Decay	2	500	1635	703	520
Downwind	No Decay	2	500	1526	440	525
Center	No Decay	6	500	545	234	173
Center	No Decay	18	500	182	78	58
Center	30 Min.	6	500	476	214	158
Downwind	No Decay	2	2500	1629	200	113
Downwind	No Decay	6	2500	543	67	38
Downwind	No Decay	18	2500	181	22	13
Downwind	*5 Min.	2	2500	3	3	2
Downwind	*5 Min.	6	2500	4	2	1
Downwind	*5 Min.	18	2500	14	2	1

* A small sample of computer calculation runs was run using a very large decay (5-minute half-life).

is the interaction between mixing ceiling and the diffusion parameter. Under a low mixing ceiling (100m) differences resulting from changes in σ_z are minimal, while under a high mixing ceiling (2500m) the diffusion parameter differences yield large differences in predicted concentrations.

The results presented here indicate that, except in the case of a very low mixing ceiling, the variations in diffusion parameter categories can result in large variations in predicted concentrations. Uncertainty exists, both in defining differences in stability categories through suitable meteorological measurements, and in relating those stability characterisitcs to specific values of diffusion parameters. In view of the demonstrated sensitivity of the model to changes in the diffusion parameter values, there is a need to develop a more definitive system which relates diffusion parameters to objectively definable meteorological characteristics.

5.4.4 Pollutant Half-Life

The effect of pollutant half-life due to atmospheric removal processes on short-term model (one-hour) concentrations was examined to determine whether it was significant, and, if so, under what conditions it was most significant. A total of 486 pairs of model inputs representing no decay and a one-half hour half-life (486 of each) were compared to examine this question. These consisted of the 972 selected combinations discussed in Section 5.4.1.

From these pairs it is found that a 30-minute half-life (a decay rate of 0.0231/min) causes a significant reduction in concentration in 45 percent of the cases. The most pronounced of these many cases are associated with relatively light wind speeds (e.g., 2 m/sec), and a receptor location which is located significantly downwind of the high emission area. The 30-minute half-life resulted in concentration reductions by a factor of 50 (98%) in the most extreme case. A selected tabulation showing variations in the effect of the decay rate with receptor location and wind speed is given in Table 28, for a 100-meter mixing ceiling with the Pasquill Class E (stable) diffusion parameters and for a 500-meter mixing ceiling with the McElroy-Pooler Class 1 (unstable) diffusion parameters.

The results show that the existence of a noticeable depletion process will have a significant effect on concentrations in the low wind situation. This effect will be especially pronounced downwind of high emission rate areas, where the effects are noticeable even at high wind speeds.

5.4.5 Wind Speed and Profile Power Law

The sensitivity of the model to wind speed measured in the city was divided into two components: the wind speed at a reference height of 20.8 meters (a convenient and representative height which corresponded to some available data), and the power which defines the vertical profile of wind speed according to the relationship:

$$u = u_1 \left(\frac{h}{z_1} \right)^p \tag{41}$$

where

u = wind speed at height h

u_1 = reference wind speed at height z_1

p = power which is a function of atmospheric stability.

Table 28. Model Concentrations With and Without a 30-Minute Decay Half-Life for Selected Combinations of Model Inputs [1]

a. Comparisons When the Mixing Ceiling is 100 m and the Diffusion Parameters are Pasquill, Class E

	Model Concentrations ($\mu g/m^3$) for Indicated Receptor Location, Wind Speed and Decay								
	Upwind			Center			Downwind		
	2 m/sec	6 m/sec	18 m/sec	2 m/sec	6 m/sec	18 m/sec	2 m/sec	6 m/sec	18 m/sec
With 30 Min. Half-Life	7	3	1	1146	478	174	41	145	134
Without Decay	11	4	1	1259	547	182	2061	687	229

b. Comparisons When the Mixing Ceiling is 500 m and the Diffusion Parameters are McElroy-Pooler, Class 1

	Model Concentrations ($\mu g/m^3$) for Indicated Receptor Location, Wind Speed and Decay								
	Upwind			Center			Downwind		
	2 m/sec	6 m/sec	18 m/sec	2 m/sec	6 m/sec	18 m/sec	2 m/sec	6 m/sec	18 m/sec
With 30 Min. Half-Life	1	1	0	412	158	56	12	41	35
Without Decay	2	1	0	520	173	58	525	175	58

(1) All Concentrations were Computed Using the St. Louis Data with 51 Point Sources, an Area Grid Mesh of 0.25 Miles, One Area Source Height and a Wind Profile Power Law of 0.15.

In the initial set of 5832 combinations of model inputs defined for the sensitivity analysis there were 2916 pairs of comparisons in which all model inputs were identical except that the power varied from 0.15 to 0.30. In none of these comparisons did the resulting concentrations vary by as much as 10 percent. As a result, this parameter was eliminated from further sensitivity consideration and a value of 0.15 was adopted as the standard value.

In the absence of decay and plume rise the insensitivity of concentrations to the power law parameter makes it clear that the model concentration is inversely proportional to wind speed. This can also be clearly seen in the model formulations. If the wind speed is constant for all emission sources (no power law effect) it can be taken outside the integral of Equation (9) and the summation in Equation (8) and becomes a common factor in the summation of Equation (10). However, the inclusion of a decay constant complicates the relationship. At the upwind and center receptor locations the effect of decay is to slightly reduce the inverse relationship. At the downwind location, the existence of decay causes a reversal in the wind speed relationship over the light to moderate wind speed range (2 to 6 m/sec). These effects are demonstrated by the results presented in Table 29.

The modeling difficulties encountered when the wind speed is of the order of 2 m/sec and less have been discussed in Section 4.2.3 of the validation analysis. To this must also be added the well known measurement problems associated with obtaining a representative value of the urban wind speed in light wind cases. While this is an infrequent occurrence (for the time periods reported in Section 4.0, winds

Table 29. Model Concentrations as a Function of Wind Speed With a 30-Minute Decay Half-Life for Selected Combinations of Model Inputs (1)

a. Comparisons When the Mixing Ceiling is 100 m

With Wind Speed of:	Model Concentrations ($\mu g/m^3$) for Indicated Diffusion Parameters, Receptor Location and Wind Speed								
	Pasquill, Class E			McElroy-Pooler, Class D			McElroy-Pooler, Class 1		
	Upwind	Center	Downwind	Upwind	Center	Downwind	Upwind	Center	Downwind
2 m/sec	7	1146	41	4	819	37	4	850	43
6 m/sec	3	478	145	2	347	147	2	364	162
18 m/sec	1	174	134	1	127	136	1	134	147

b. Comparisons When the Mixing Ceiling is 500 m

With Wind Speed of:	Model Concentrations ($\mu g/m^3$) for Indicated Diffusion Parameters, Receptor Locations and Wind Speed								
	Pasquill, Class E			McElroy-Pooler, Class D			McElroy-Pooler, Class 1		
	Upwind	Center	Downwind	Upwind	Center	Downwind	Upwind	Center	Downwind
2 m/sec	7	1143	36	2	554	11	1	412	12
6 m/sec	3	476	109	1	214	32	1	158	41
18 m/sec	1	173	100	0	76	29	0	56	35

(1) All Concentrations were Computed Using the St. Louis Data with 51 Point Sources, an Area Grid Mesh of 0.25 Miles, One Area Source Height and a Wind Profile Power Law of 0.15.

were 2 m/sec and less in St. Louis 1.5% of the time, and in Chicago, 6% of the time), it remains a subject for further study from both the modeling and the measurement points of view.

5.4.6 Mixing Ceiling

The sensitivity of model concentrations to changes in the mixing ceiling was examined using mixing ceilings of 100, 500 and 2500 meters. Effects associated with 486 pairs of comparisons of 100- and 500-meter ceiling heights were examined based on the 972 input combinations obtained as described in Section 5.4.1. The most pronounced influence was observed for diffusion parameters associated with unstable meteorological conditions (McElroy, Class 1). The least pronounced influence was observed for diffusion parameters associated with stable meteorological conditions (McElroy-Pooler, Class 1). The least pronounced locations where minimal travel from the principal effective source region was involved. These effects may be clearly discerned in the selected results listed in Table 30. In addition to the 100-and 500-meter mixing ceilings, results from a 2500-meter ceiling have been added for the downwind receptor. These results show that under stable conditions the increased mixing ceiling has no effect, but under neutral and unstable conditions a noticeable effect occurs. These results suggest that, at downwind locations where significant travel from the primary emission area is involved, the concentration is nearly inversely proportional to the mixing ceiling. With increasingly stable diffusion parameters this effect is reduced until with the stable type of diffusion parameter the effect of the mixing ceiling is negligible.

Table 30. Model Concentrations as a Function of Mixing Ceiling With a Wind Speed of 6 m/sec for Selected Combinations of Model Inputs (1)

a. Comparisons When there is No Decay

With Mixing Ceiling of:	Model Concentrations ($\mu g/m^3$) for Indicated Diffusion Parameters, Receptor Location and Mixing Ceiling								
	Pasquill, Class E			McElroy-Pooler, Class D			McElroy-Pooler, Class 1		
	Upwind	Center	Downwind	Upwind	Center	Downwind	Upwind	Center	Downwind
100 m	4	587	687	3	402	698	3	425	748
500 m	4	545	509	2	234	147	1	173	175
2500 m	---	---	509	---	---	67	---	---	38

b. Comparisons When the Decay Half-Life is 30 Minutes

With Mixing Ceiling of:	Model Concentrations ($\mu g/m^3$) for Indicated Diffusion Parameters, Receptor Location and Mixing Ceiling								
	Pasquill, Class E			McElroy-Pooler, Class D			McElroy-Pooler, Class 1		
	Upwind	Center	Downwind	Upwind	Center	Downwind	Upwind	Center	Downwind
100 m	3	478	145	2	347	147	2	364	162
500 m	3	476	109	1	214	32	1	158	41

(1) All Concentrations were Computed Using the St. Louis Data with 51 Point Sources, an Area Source Grid Mesh of 0.25 Miles, One Area Source Height and a Wind Profile Power Law of 0.15.

In general, the results obtained indicate that the pollutant concentrations are approximately inversely proportional to the mixing ceiling (as defined in these calculations) under conditions which reflect greatest sensitivity. Under such conditions this result is in agreement with the predictions of a box model, in which the pollutant is uniformly dispersed in the vertical. Under stable conditions, or when the predominant pollutant travel distances are small, the model is less sensitive to the mixing ceiling. Under the defined sensitive conditions the model is thus subject to prediction errors associated with inaccuracies in mixing ceiling estimates. Inaccuracies will occur in the presently used, rather indirect methods by which hourly variations in ceiling heights must be estimated with currently available meteorological data.

5.4.7 Wind Direction

The influence of wind direction is most critical with regard to specific receptor locations which may, or may not be, influenced by a strong upwind source, depending on small variations in wind direction. Thus, receptor locations in the center of a strong emission area are equally affected by all wind directions, while locations outside a strong emission area are strongly influenced by whether they are directly downwind of the high emission area.

The effect of various possible errors in wind direction on short-term concentrations was tested using the emission data discussed in Section 5.2. The effect of errors in the wind direction estimate of 3, 10 and 45 degrees was examined for the two wind directions shown previously in Figure 44. The error was allowed to vary to either side of the true direction, and the absolute values of the resulting errors in concentration were averaged for summarizing purposes. Resultant concentrations were evaluated at the three selected receptor locations shown in Figure 44, using combinations of the following parameter values:

Parameter	Value
wind speed	2, 6 and 18 m/sec
mixing ceiling	100 and 500 meters
diffusion parameters	Pasquill Class E; McElroy-Pooler Class D; McElroy-Pooler Class 1
decay half-life	no decay
wind profile exponent	0.15
number of point sources	51
area source grid spacing	0.25 miles
distribution of area source emission heights	all at 30 meters

Table 31 contains selected results for the case where all sources (area and point) are considered, and the wind is first taken to be from 349° (Table 31a) (few large upwind point sources; see Figure 44), and then from 020° (Table 31b) (many large upwind point sources). The other fixed conditions are a neutral atmosphere stability and a 500 meter mixing ceiling. The results for the 349-degree direction (Table 31a) demonstrate the variations in model concentration which can occur with various values of wind error, and show the change in effect of such an error depending upon the specific receptor location considered. Errors can go as high as about 25 percent at the central receptor, and up to

Table 31. Model Concentrations with Various Degrees of Error in the Wind Direction Estimate for Selected Combinations of Model Inputs (1)

a. Comparisons when the Wind Direction is 34[illegible] (See Figure 44)

	Model Concentrations ($\mu g/m^3$) and Absolute Errors for Indicated Receptor Location and Wind Speed								
	Upwind			Center			Downwind		
	2 m/sec	6 m/sec	18 m/sec	2 m/sec	6 m/sec	18 m/sec	2 m/sec	6 m/sec	18 m/sec
Model Concentration: No Wind Error	3	1	0	603	201	67	469	156	52
Absolute Error in Model Concentration: With 3 Degree Wind Error	0	0	0	76	25	8	80	27	9
10 Degree Wind Error	1	0	0	73	24	8	227	76	25
45 Degree Wind Error	28	9	3	143	48	16	445	148	49

b. Comparisons when the Wind Direction is 020° (See Figure 44)

	Model Concentrations ($\mu g/m^3$) and Absolute Errors for Indicated Receptor Location and Wind Speed								
	Upwind			Center			Downwind		
	2 m/sec	6 m/sec	18 m/sec	2 m/sec	6 m/sec	18 m/sec	2 m/sec	6 m/sec	18 m/sec
Model Concentration: No Wind Error	7	2	1	1055	352	117	23	8	3
Absolute Error in Model Concentration: With 3 Degree Wind Error	12	4	1	227	76	25	18	6	2
10 Degree Wind Error	18	6	2	716	239	80	154	51	17
45 Degree Wind Error	75	25	8	308	103	34	125	42	14

(1) All concentrations were computed using the St. Louis data with 51 point sources, an area grid mesh of 0.25 miles, one area source height, a wind profile power of 0.15, neutral atmospheric stability and a 500 m mixing ceiling.

100 percent at the downwind location. Note that the pattern is consistent at the downwind location (increasing concentration error with increasing wind error), but not at the central site. Changes in the stability condition (to unstable, or to stable) and/or the mixing ceiling (to 100m) show different absolute values of concentration and error, but quite similar patterns. The results in Table 31b for the 020° direction should be interpreted bearing in mind that this wind shift consideration transfers the relative locations of the up- and downwind sites to some extent in the acrosswind direction (see Figure 44). Errors at the central site can now become significantly larger (up to about 70%) because of the significant upwind point sources, and the other two sites show increased errors, with the "downwind" site losing the consistent increase in error with increased direction error which it had in Table 31a.

These results show the extreme variability of this effect, and the importance of obtaining a representative wind direction to enable adequate definition of the individual short-term concentrations at certain specific types of site locations.

For long-term concentrations, errors associated with the mean wind direction during any given period tend to be compensated for during other periods, when a sufficiently large sample is used to construct the long-term mean and frequency distribution of short-term concentrations. The use of a statistical sampling plan to select wind directions in constructing long-term averages obviates the need for considering the problem of defining an appropriate class interval size for characterizing wind directions in a long-term concentration model. The results of statistical sampling plan evaluation discussed in Section 4.3.2 show that long-term concentrations consturcted using an unbiased sample of about 100 short-term periods will properly reflect the effects of wind direction variations.

5.4.8 Diurnal Variation in Emission Rates

The sensitivity of the model to diurnal variations in SO_2 emission rates is evaluated in this section by analyzing the factors which affect the emission rate estimations. These factors are represented in algorithms which are used to define the spatial distribution of emissions for any given hour and the variations of the emissions from hour to hour. The algorithms used in the validation analysis of this study to represent St. Louis and Chicago emissions are given in Appendixes B and C, respectively. The inputs to these algorithms which vary diurnally, and thus give rise to the diurnal emission variations, are temperature, electric power load at generating stations, and hour of the day. Since the errors associated with measurement of these inputs are small, it is clear that the errors which are more critical to model sensitivity are those associated with the assumptions in the emission algorithms which convert these inputs into the distributions of SO_2 emissions. In the discussion which follows, these sources of error and their impact on model calculations are identified and characterized.

Sulfur dioxide emissions are characterized as arising from one of three types of operations, namely, space heating, electric power generation, and industrial processing. All three operations emit SO_2

as a result of fuel consumption. However, industrial processing may also include some direct emissions of SO_2. The amount of annual emissions associated with each type of operation for each point source and each subdivision of an area source is determined from emission inventory surveys. These surveys may provide more detailed breakdowns including seasonal or even monthly emissions. These annual (or other more frequent) values of emissions determine the spatial distribution of emissions by type of operations. These emission estimates also act as scaling factors for diurnal variations which are applied to each type of operation. Thus, they determine the magnitude of the diurnal variation at each location. An error in one of the estimates creates a systematic error in the model predictions for locations in the vicinity of the error estimate. However, the occurrence of this type of error will be distributed randomly over all sources. If concentrations are considered at a number of locations widely dispersed over the urban area, the overpredictions and underpredictions due to this type of error will tend to balance at any given time.

Diurnal variations in emissions from electric power generation are estimated by means of linear relationships with hourly electric power loads of specific generating units (e.g., see Section 4.1). The error associated with these estimates is small. The uncertainty of emission estimates for proposed power plants would be greater. However, the emission rate estimates for this type of operation are judged to be sufficiently well represented that they have less impact on model sensitivity than other errors which need to be considered.

Diurnal variations in emissions from industrial processing are allocated on the basis of scaling factors which define the percent of the peak operating capacity which is applicable to each day of the week and to each eight-hour shift of the day. The algorithms used for St. Louis and Chicago allow for three types of days of the week, namely, weekday, Saturday, and Sunday or holiday. An input to the algorithm designates the type of day which is assigned to each particular hour for which a set of emission rates is requested. In the Chicago case, sufficient data were collected on each point source to assign a specific type of day to each day of the week. For example, for some sources every day is treated as a weekday, and for some other sources, Monday is designated as a holiday. For national holidays, all sources are assigned holiday schedules. During any particular day and hour, variations in actual emissions from these scheduled average emissions may be considerable. This is because industrial operations must respond to fluctuations in demand and to breakdowns in equipment. These influences will result in errors in emission rate estimates in the immediate vicinity of individual sources. However, it is probable that these errors will be randomly distributed over an urban area at any given time. When concentration predictors are considered over a number of widely dispersed locations, the overprediction and underprediction errors will tend to balance. Only detailed analysis of production records of individual plant operations can be expected to yield more accurate emission estimates.

Emissions from space heating operations reflect diurnal cycles in demand for heat and in temperature fluctuations. While these two factors tend to have opposite diurnal cycles, the resulting diurnal pattern of heating operations is rarely uniform. The emission rates for space heating operations are estimated by the following equation:

$$Q(t) = q_T \, [T_R - T(t) - \Delta(t,d)], \qquad [T(t) + \Delta(t,d)] \leq T_R \quad (42)$$

where

$Q(t)$ = emission rate for time t

q_T = emission rate per degree

T_R = reference temperature (usually 65°F)

$T(t)$ = temperature for time t

$\Delta(t,d)$ = temperature correction for time t and type of day d.

The temperature correction is an empirical factor to account for the diurnal variation in the activities of a city which affect its demand for fuel. Corrections were determined for St. Louis for each hour of the day for weekdays, Saturdays and Sundays by Turner (1968). Two sets of correction factors were derived. One is applicable to residential space heating. The other is applicable to commerical and industrial space heating. A further correction has been applied to emissions for the Chicago area where residential heating emissions were borken down between large apartment buildings (20 dwelling units or more) and small apartment buildings and residences (low-rise). A stoking factor, or "janitor" function, which permits no emissions from 11 p.m. to 5 a.m.

(3 a.m. if the temperature is below 5°F), and requires a 50 percent excess for the first two hours of the day (recommended by Roberts, et al., 1970) was applied to low-rise residential emissions.

Random errors associated with individual sources of these types may be expected. However, these are probably small. A more serious type of potential error is associated with assumptions regarding the response of such emissions to sudden temperature changes and to unseasonal temperatures. This type of error will be systematic and city-wide. For example, since buildings provide insulation between outside air and inside air, there will usually be a significant time lapse between a sudden temperature change and the time when its influence on inside air requires full compensation by increased fuel consumption. However, the emission algorithm assumes this adjustment takes place immediately. The effect of this lag on fuel consumption was pointed out by Turner (1968). His findings for a severe temperature change of 15°F in one hour suggest that a six to eight hour period of adjustment is required. The error in emission rates during the hour in which the change occurs is shown in Turner's example to be factor of two too high and to return to no error in six to eight hours. While this type of error is critical to short-term model sensitivity, it is not important for long-term mean concentrations because sharp temperature changes are rare over a long period.

Systematic errors due to unseasonal temperatures can also result from the fact that many heating systems, especially in large buildings, are only partially controlled by temperature thermostats. Large amounts of excess heat may be generated when the temperature is unseasonably warm, and the emission estimate will be, correspondingly, too low. Similarly, insufficient heat will be generated during unseasonably cold periods, with an emission overestimate. This type of error will persist for periods of several hours to several days depending on the duration of the unseasonable temperatures. These errors should tend to compensate each other over long-term periods. However, systematic errors will exist in short predictions and, because the contribution of these sources frequently represents most, or all, of the affected concentration, the concentration error will be directly proportional to the emission error. A careful study of the magnitude and duration of heating emissions is required to determine the nature of heating system response to these types of situations.

It is concluded that mean long-term concentrations are not sensitive to errors in the diurnal variations in emission rates. However, it is clear that individual short-term concentrations will be proportionally sensitive to significant errors in the diurnal variation factor. During winter seasons, when ground level concentrations are primarily due to emissions from space heating operations, the short-term concentrations may be in error by as much as a factor of two due to errors in temperature dependent emission rates.

5.5 FINDINGS

A summary of the preceding results on the sensitivity of the Gaussian plume type of multiple source urban diffusion model is given below. These results are based on calculated changes in short-term concentrations at a point associated with changes in model inputs. Three types of receptor locations are considered within a selected representative pattern of urban area source emissions. Combinations of two or three values for each of 10 input parameters were examined in drawing conclusions regarding the sensitivity of the model. A change in concentrations at a point of at least 50 percent due to a change in an input value was considered a "sensitive" effect. Sensitivities in many cases are complex and interrelated, and the individual section analyses should be consulted for details.

The sensitivity findings for each input parameter are summarized as follows:

- Spatial Variability of Emissions. The fineness of the grid spacing used to represent area sources must be consistent with the dimensions of real spatial variability. For example, if the standard deviation of emission rates defined by quarter-mile squares is as much as 50 percent of the mean emission rate for a square-mile, a change from a grid spacing of a mile to a quarter-mile produces "sensitive" changes. Furthermore, when a small grid spacing is used, large individual sources may be aggregated into the area source without producing "sensitive" changes.

- Vertical Distribution of Area Source Emissions. On the basis of comparisons between concentrations calculated using a single height for area source emissions, with concentrations calculated using a distribution of heights (50% of emissions at mean height, 25% at one-half the mean height and 25% at 1.5 times the mean height), it is concluded that this is not a "sensitive" input. No "sensitive" changes were observed in the comparisons.

- Vertical Diffusion Parameter. Under conditions which do not involve low (e.g., 100m) mixing ceilings, calculated short-term concentrations were shown to vary by a factor of from 3 to 10 or more when the diffusion parameters are varied from the Pasquill Class E to the McElroy-Pooler Class 1 (stability classes defined in Section 2.4.4). This large sensitivity indicates the need for measurements of atmospheric conditions which are clearly related to differences in diffusion conditions (i.e., values of σ_z).

- Pollutant Half-Life. In order to adequately estimate concentrations at locations downwind of major emission areas, information on the pollutant half-life due to atmospheric removal processes must be available. As an extreme example of the wide spectrum of comparisons obtained, highly significant effects were computed for a location 30 km downwind of the center of the urban area when comparing no decay with a 30-minute half-life. Concentrations with no decay were 50 times greater than concentrations with decay.

- Wind Speed and Profile Parameter Value. Calculated concentrations are insensitive to changes in the wind profile power law exponent. Maximum changes in calculated concentrations were 10 percent when the exponent was varied from 0.15 to 0.3. Calculated concentrations are inversely proportional to wind speed when pollutant decay is negligible. Decay acts to reduce the "sensitivity" effect due to wind speed at locations downwind of the primary emission area.

- Mixing Ceiling. Changes in the mixing ceiling produce the greatest sensitivity at locations for which most of the pollutant arrives after traveling large distances. At locations 30 km downwind from the primary emission area, the calculated concentration varied inversely with the mixing ceiling in unstable conditions. This maximum "sensitivity" effect decreases with increasing stability and is negligible in stable conditions.

- Wind Direction. A highly variable sensitivity exists for short-term single station concentrations. Small changes in wind direction (e.g., 3° azimuth) may result in extremely "sensitive" effects at some locations. Short-term concentration estimates are thus dependent on accurate wind direction estimates.

- Diurnal Variation in Emission Rates. Errors in reported annual or seasonal emissions from particular sources will result in proportionally systematic errors in calculated diurnal variations in concentrations in the vicinity of the emission error. Because the emission algorithms are temperature based, unseasonable temperatures or sudden atmospheric temperature changes will result in corresponding systematic errors in predicted short-term concentrations at all locations for a short lag period, until an adjustment in space heating operations occurs. Over a long-term period errors in short-term concentrations due to differences between actual and estimated emission rates will tend to be balanced in the combined frequency distribution of short-term concentrations for several locations.

- Long-Term Concentrations. Sensitivity of the long-term model is defined as it relates to the model described in Section 4.3. Errors in model inputs will include the sensitivity effects summarized above for short-term concentrations. However, over a long-term period the random errors tend to compensate each other. It is evident that this is reasonably true for model inputs used for validation analysis in this study, since long-term concentration calculations averaged over several locations were generally found to be in agreement with observed concentrations. Furthermore, the combined frequency distribution of observed short-term concentrations at all locations considered were well represented by the model calculations.

  The long-term model can be expected to show comparable sensitivity to some but not all, of the systematic (as opposed to random) changes in the parametric inputs described above for the short-term model. Those which can impact are the spatial variability of emissions, the vertical diffusion parameter selection, pollutant half-life, wind speed and mixing ceiling.

Section 6.0

CONCLUSIONS AND RECOMMENDATIONS

Section 6.0

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The results of this evaluation of the validity and the sensitivity of the Gaussian plume type of urban diffusion model provide basic definition of the capabilities and limitations of the model for simulating urban air quality. The following represent the important conclusions derived from the validation and sensitivity findings, respectively.

6.1. CONCLUSIONS FROM VALIDATION ANALYSIS

From the findings in the validation study in which comparisons are made with data from two cities for one and three month periods, and the model is implemented as described in Section 4.0, it is concluded that:

1. For individual values of short-term (1- or 2-hour) concentrations at individual receptor locations, the predicted concentrations show large deviations from the observed concentrations. However, a large number of such comparisons over a month, or a season, produce frequency distributions of predicted concentrations which compare quite well with the observed distributions. The individual frequency deciles are generally within a factor of two or less of each other. No single controlling factor could be found which consistently accounted for a significant fraction of the deviations of the individual short-term values.

2. Predicted long-term (monthly or seasonal) concentrations based on averaging of the calculated short-term concentrations, show consistent good agreement with observations, with a root-mean-square error equal to about half the mean, and a slight tendency to overestimate. This contrasts with results from other long-term models which generally overestimate significantly; the improvement is concluded to be largely due to the combination of two factors, one being the process of accounting for the diurnal correlation of meteorological and emission parameters, and the other, the use in this model of urban-derived diffusion parameters (McElroy-Pooler parameters based on the Turner stability classifications).

3. A technique has been devised for calculating the long-term estimates described above without the necessity of calculating every short-term concentration involved. This is the statistical process of proportionate stratified sampling, and is an effective method for selecting a limited set of short-term periods which adequately define the distribution in the long-term period. As few as 5 to 10 percent of the total number of short-term periods involved will describe the distribution adequately, if the sampling is done as described in Section 4.3.2.

As noted in Section 4.2.3, the calm or light wind case represents a special problem; while suggestions for empirical treatment are given in that section, the subject requires further study.

6.2 CONCLUSIONS FROM SENSITIVITY ANALYSIS

From the findings in the sensitivity analysis, it is concluded that, generally, concentrations predicted by the short-term model were found to be insensitive to changes in the vertical distribution of area source emissions and the wind profile parameter value. The concentrations are sensitive, under some circumstances, to changes in spacial variability in emissions, vertical diffusion parameter, pollutant half-life, wind speed, mixing ceiling, wind direction and diurnal variation in emission rates. The long-term model (defined in Section 4.3) is sensitive in some cases to the spatial variability of emissions, vertical diffusion parameters, pollutant half-life, wind speed and mixing ceiling.

More specifically, selected principal sensitivity results are as follows:

1. A fine grid spacing (0.25 mile on a side) is necessary for area source definition if the emissions vary significantly over a square mile (standard deviation of emission rates as much as 50 percent of the mean). Conversely, if a coarse grid spacing is used, then more care must be taken in determining the significant point sources to be considered.

2. The model shows sensitivity to selection of the stability class assigned in any given calculation of short-term concentration, and additionally, overall sensitivity to the choice of one set of diffusion parameters (e.g., McElroy-Pooler) over another (e.g., Pasquill).

3. When pollutant decay is negligible, the model shows an inverse proportionality relationship with wind speed; in the presence of a pollutant half-life of 30 minutes, the variations of concentration with wind speed at downwind locations are markedly reduced.

4. Mixing ceiling shows its maximum effect in terms of sensitivity at large downwind distances under stable conditions.

5. Sensitivity to wind direction is highly variable, and of course shows the most impact at individual stations downwind of major sources.

6. Diurnal variations in emission rates are governed in the model algorithms by air temperatures, and in unseasonably warm or cold periods will result in proportionate over- or underestimates of emissions, and hence concentrations; these will exist for a short (several hours to several days) period, gradually recovering to correct the emission values.

6.3 RECOMMENDATIONS

On the basis of this study, it is recommended that:

1. Consideration should be given to EPA's promulgation, for general use, of the long-term version of the Gaussian plume type of urban diffusion model described in this report, using the proportionate stratified sampling concept, for the calculation of long-term means and short-term distributions of pollutant concentrations. Appropriate documentation should be prepared, together with processing procedures for meteorolgical and emission inputs, and program manuals for an optimized computer program (to be developed).

2. Study should be instituted on the various measurement and classification problems described in this report, particularly (1) the relationship of the appropriate meteorological measurements to the corresponding stability categories, (2) mixing ceilings, and (3) wind directions. In addition, the calm or light wind case should be studied to to determine a satisfactory and objective method of predicting pollutant concentrations under these circumstances.

Section 7.0

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Appendix A

A SUMMARY OF PREVIOUS IMPLEMENTATIONS OF THE GAUSSIAN PLUME TYPE OF URBAN DIFFUSION MODEL

This appendix contains summaries of implementations of the Gaussian plume model to analyze pollutant concentrations from multiple sources in an urban environment. The summaries include:

- Scope of application addressed by the investigator
- Treatment given to emission data
- Computational equations used
- Meteorological and other non-source data
- Validation results obtained.

The implementations summarized are identified by the name of the investigator and indexed by exhibit number as follows:

Investigator	Exhibit
Lucas (1958)	A-2
Pooler (1961)	A-3
Turner (1964)	A-4
Clarke (1964)	A-5
Miller & Holzworth (1967)	A-6
Koogler, et al. (1967)	A-7
Martin & Tikvart (1968)	A-8
Fortak (1969)	A-9
Milford, et al. (1970)	A-10
Ludwig, et al. (1970)	A-11
Calder (1970)	A-12
Singer & Smith (1970)	A-13

A list of the symbols used in the summaries is presented as Table A-1. Symbols used only with regard to one investigator's work are introduced as they are encountered.

The descriptions here are not comprehensive in that they do not attempt to present or discuss all the investigator's findings. The summaries present the basic method used to implement the model and the results of validating this model. Further results obtained by fitting the model to data or examining the effect of additional refinements beyond the scope of the basic model are not discussed.

Table A-1. Symbols

Symbol	Explanation
$\overline{C}$	Seasonal or long-term mean concentration over a sequence of short-term (steady-state) periods
C_A	Concentration due to area sources
C_p	Concentration due to point sources
C or C_k	Short-term (steady-state) concentration
q, q_o	Emission rate per unit area (area source)
Q, Q_i	Emission rate (point source)
V	Stack effluent velocity (point source)
D	Stack diameter (point source)
T_s	Stack effluent temperature (point source)
H, H_i	Physical height of source
ΔH, ΔH_i	Plume rise
h, h_i	Effective source height
S	Alongwind length of area source
x, x_i, r, r_i	Alongwind distance between source and receptor locations
y, y_i	Crosswind distance between source and receptor locations
θ_i	Azimuth from receptor to source
θ	Mean wind direction
u	Mean wind speed
u_j	Representative wind speed for jth wind speed class
K	Empirical diffusion parameter

(Continued)

Table A-1. Symbols (Concluded)

Symbol	Explanation
f( )	Frequency distribution of specified variables
L, L_k	Mixing layer depth or ceiling
T	Ambient air temperature
t_{50}	Pollutant airborne half-life
t, t_i	Travel time from source to receptor with mean wind speed
σ_y, $(\sigma_y)_i$	Horizontal diffusion parameter
σ_z, $(\sigma_z)_i$	Vertical diffusion parameter

Exhibit A-2. Model Implementation by Lucas (1958)

I. Scope:

Short-term and seasonal mean concentrations from domestic fires in an urban area.

II. Treatment of Sources:

Represent emissions by a uniform area source (i.e., q, S and h) for London

$$q = 1.7 \times 10^{-8} \frac{ft^3 SO_2}{ft^2 sec} \quad \text{(1954 estimate)}$$

Under "normal" meteorological conditions

$$h = 30 + 5 \left(\frac{3}{u}\right)^3$$

Under stable meteorological conditions

u, ft/sec	≤ 1	2	3	≥ 5
h, ft	80	45	35	30

III. Computational Equations:

Approximate a Gaussian plume for a point source by a uniform cone (allowing for impenetrability of the ground and mass continuity) and integrate the resulting equation over the source area to get concentration as a function of distance from the upwind edge of the source area. For short-term with $x \leq S$,

$$C_1(x) = \frac{q}{\sqrt{\pi}\, Ku} \left\{ \ln \frac{K^2 x^2}{h^2} + \frac{h^2}{K^2 x^2} - \frac{h^4}{K^4 x^4 (2)2!} + \frac{h^6}{K^6 x^6 (3)3!} - \ldots \right\}$$

With $x > S$,

$$C_2(x) = C_1(x) - C_1(x - S)$$

Estimate long-term concentrations using short-term concentrations associated with wind speed classes as follows,

$$\overline{C}(x) = \sum_j f(u_j)\ C_k(x).$$

IV. Meteorological Parameters:

Use mean wind speed or frequency distribution of wind speed classes. The diffusion parameter K is 0.041 for "normal" conditions; 0.014 for stable conditions (based on ft, sec unit system). Use normal value for long-term estimates.

V. Validation Results:

Pollutant, Location, Time	Observed	Calculated
SO_2, London, 1954-55 winter season	0.114 ppm	0.11 ppm
SO_2, London, 5-8 Dec., 1952	1.5 ppm	9.0 ppm(a)

(a) A two-level diurnally varying emission rate (i.e., constant for 15 hours, zero for 9 hours) was used in this prediction. The calculation as presented graphically by Lucas appears to be related to a puff, rather than a plume, type of calculation in which emissions during one period are traced during the succeeding period in which zero emissions occur. The details of the calculation are not reported.

Exhibit A-3. Model Implementation by Pooler (1961)

I. Scope:

Mean monthly pollutant concentrations resulting from multiple pollutant sources at a gridwork of receptor locations.

II. Treatment of Sources:

Represent emissions (Q) from each square mile of an urban area by a point source in the center. Treat all emissions as having an effective height of 30 m. Receptor concentrations are calculated for the same locations used as point sources. Emissions (q_0) from the square centered on a receptor are treated as a uniform circular area source.

III. Computational Equation:

Treat the plume from a point source as having a Gaussian distribution of pollutant concentrations in the vertical and a uniform distribution over a sector of angle $\pi/8$ in the horizontal (allowing for impenetrability of the ground and mass continuity). Let $f(u_j, \theta)$ denote the relative frequency of occurrence of a wind speed class with an average value of u_j and a wind direction class with median value θ. The concentration per unit emission rate at a receptor, due to emissions from a point source a distance x_i and azimuth θ_i from the receptor is:

$$R(\theta_i) = \sum_j \frac{2f(u_j, \theta_i)}{\sqrt{2\pi}\,(\frac{\pi}{8})\, x_i u_j \sigma_i} \exp\left(-\frac{h^2}{2\sigma_i^2}\right)$$

where

$$\sigma_i = 2Ku_j^{\alpha-\beta}x_i^{\beta}$$

α, β = empirical diffusion parameters.

Over a circular area source of 1 mi^2 the concentration per unit emission rate per unit area is:

$$R_o = \frac{2}{\sqrt{2\pi}} \sum_j \frac{f(u_j)}{u_j} \int_0^{.908} \frac{1}{\sigma} \exp\left(-\frac{h^2}{2\sigma^2}\right) dx$$

Use linear interpolation between wind direction class medians to obtain the concentration due to each source and sum,

$$\overline{C} = q_o R_o + \sum_i Q_i \left\{R(\phi_i) + \frac{8}{\pi} \left|\theta_i - \phi_i\right| \left[R(\psi_i) - R(\phi_i)\right]\right\}$$

where

ψ_i = clockwise most adjacent wind direction class median
ϕ_i = anticlockwise most adjacent wind direction class median
θ_i and ϕ_i are in radians.

IV. Meteorological Parameters:

Joint frequency distributions of wind speed classes having average values of u_j and wind direction classes having median values of θ are required to be known for the period of interest. Over periods of a month the following values of the meteorologically oriented diffusion parameters were used for Nashville, Tennessee: $\alpha = 0.6$, $\beta = 1.5$, $K = 0.06$.

V. Validation Results:

An analysis of the regression of observed monthly lead peroxide candle sulphation rate on concentrations derived by interpolating isopleths drawn for the gridwork of calculated mean monthly concentrations was made for available data from 123 sampling locations in Nashville, Tennessee, for the months of November 1958 through March 1959. One-half of the observed concentrations were reported to be between 80 and 125 percent of the regression relationship. Less than 5 percent of the observed values deviated from the regression relationship by more than a factor of two.

Exhibit A-4. Model Implementation by Turner (1964)

I. Scope:

Estimate 24-hour gaseous pollutant concentrations (e.g., SO_2) as the mean of calculated 2-hour steady state concentrations at a gridwork of receptor locations in an urban area.

II. Treatment of Sources:

Represent emissions from each square mile of a rectangular gridwork covering the urban area source by a normal line source centered on the square, oriented perpendicular to the wind, having a standard deviation (σ) of 402m and having an emission rate Q_i. Treat all source emissions as having an effective height (h) of 20m. Use available data to estimate emission rates for specific periods (e.g., 6 A.M. to 8 A.M., Nov. 12, 1958).

III. Computational Equations:

A. For short-term steady state,

Represent the emissions from each normal line source as a Gaussian plume (allowing for impenetrability of the ground and mass continuity) using a modification of the Pasquill diffusion parameters σ_y and σ_z (see meteorological parameters). Treat SO_2 as being subject to exponential decay with a half-life (t_{50}) of 4 hours. Sum concentrations from all sources.

$$C = \sum_i \frac{Q_i}{\pi u (\sigma_y)_i (\sigma_z)_i} \exp \left\{ -\frac{1}{2} \left[\frac{y_i^2}{(\sigma_y)_i^2} + \frac{h^2}{(\sigma_z)_i^2} \right] - \frac{0.693\, t_i}{t_{50}} \right\}$$

B. For long term,

Divide long-term period (e.g., 24 hours) into short-term quasi-steady state periods (e.g., 2 hours) and compute mean of steady state estimates, e.g.:

$$\bar{C} = \frac{1}{12} \sum_{k=1}^{12} C_k$$

IV. Meteorological Parameters:

Determine mean wind speed, wind direction and atmospheric stability class for each short-term period. Stability classes are defined as described in preceding text (see Tables 2 and 3). Using a wind speed of 5 m/sec, the Pasquill diffusion parameters (σ_y' and σ_z) were converted to functions of time and stability class (see Turner, 1964). Use t_i and these realtionships to get $(\sigma_z)_i$ and $(\sigma_y')_i$. Then, $(\sigma_y)_i = \sigma + (\sigma_y')_i$.

V. Validation Results:

Calculated concentrations were estimated for sampling locations by interpolating from an isopleth analysis of initial calculated values. In 1036 comparisons (available from 32 locations and 35 24-hour periods without precipitation, in Nashville, Tennessee) the following results were obtained for calculated and observed concentrations rounded to nearest pphm.

Number of zero differences	263
Number of 1 pphm differences	602
Average absolute error	2.06 pphm
Root mean square error	3.28 pphm
Skill score	0.13

In 2707 comparisons of 2-hour concentrations (7 sampler locations) selected from the same period it was noted that 43.7% of the differences were within 1 pphm.

Exhibit A-5. Model Implementation by Clarke (1964)

I. Scope:

Utilize accepted diffusion coefficients and readily available meteorological data in a simple model not requiring an electronic computer to estimate average daily urban pollution concentrations and diurnal variations.

II. Treatment of Sources:

Estimate short-term emission rates of significant point sources (e.g., 2-hour rate for power plants; however, Clarke was only able to obtain a constant emission rate for a single significant Cincinnati power plant, i.e., 77 tons/day of SO_2 and 4 tons/day of NO_x). Using emission inventory data grouped by homogeneous areas, estimate zero, average and maximum degree day emission rates for each subdivision of a circular gridwork of model oriented areas centered on a receptor location. Use daily degree day observations to interpolate between these values. To define the diffusion model oriented areas, determine the radial distances r_1, r_2, r_3 and r_{max} which for $Q_i = 1$ and $u = 1$ satisfy:

$$\int_{o}^{r_1} C_A \, dx = \int_{r_1}^{r_2} C_A \, dx = \int_{r_2}^{r_3} C_A \, dx = \int_{r_3}^{r_{max}} C_A \, dx$$

For a given stability class these integrals are functions of distance only and the divisions may be determined graphically. Wind direction class sector lines and the radial distances define the area subdivisions. For the area source H = 30m for SO_2 and 20m for NO_x. For point sources the plume rise is given by the Davidson-Bryant formula (e.g., see Briggs 1969, p.23) and $h_i = H_i + \Delta H_i$.

III. Computational Equations:

A. For short-term concentrations $C_k = C_p + C_A$

$$C_p = \sum_{i=1}^{N} \frac{2\,Q_i}{u\sqrt{2\pi}\left(\frac{\pi}{\delta}\right)\, x_i (\sigma_z)_i} \exp\left\{- \frac{h_i^2}{2(\sigma_z)_i^2}\right\}$$

where N = number of point sources whose azimuth from receptor to source lies within the prevailing wind direction class.

$$C_A = \sum_{i=1}^{4} \frac{2\,Q_i}{u\sqrt{2\pi}\left(\frac{\pi}{\delta}\right)\, x_i (\sigma_z)_i} \exp\left\{- \frac{h^2}{2(\sigma_z)_i^2}\right\}$$

where Q_i = emission rate of ith sector segment for sectors lying within prevailing wind direction class

$x_i = \sqrt{\frac{1}{2}(r_i^2 + r_{i-1}^2)}$ = source to receptor alongwind distance ($r_0 = 0$)

B. For long-term concentrations, compute the mean of the N component short-term period concentrations, e.g.:

$$\overline{C} = \frac{1}{N} \sum_{k=1}^{N} C_k$$

IV. Meteorological Parameters:

For each quasi steady-state period determine the wind direction class, wind speed and Turner (1964) stability category (e.g., see Tables 2 and 3 of text).

Use Turner's (1964) graphs to determine σ_z values as functions of the stability category and travel time t_i.

V. Validation Results:

Comparing 19 observed and calculated 24-hour concentrations for Cincinatti:

	CAMP Station		Kettering Laboratory
	NO_x	SO_2	SO_2
Number of differences of 2 pphm or less	14	18	
Number of calculations within a factor of 2 of observations	18	15	
Regression of observed on calculated values (pphm)			
Correlation coefficient	0.67	0.71	0.81
Slope	0.66	0.42	0.34
Intercept	3.4	1.1	0.45

Exhibit A-6. Model Implementation by Miller and Holzworth (1967)

I. Scope:

Maximum and average short-term concentrations over a metropolitan area without the use of an electronic computer.

II. Treatment of Sources:

Represent emissions as a continuous and uniform area source with infinite crosswind dimension and a ground-level source height.

III. Computational Equations:

Treat area source as a continuum of infinite crosswind line sources, each with emission rates q dx. Represent the plume from each line by a vertical Gaussian distribution down to the distance where 1.25 times the diffusion parameter σ_z equals the mixing layer ceiling (i.e., travel time t_L); beyond this distance use a uniform vertical distribution. Only emissions with a travel time of 50 seconds or more are considered at any receptor.

A. Maximum concentration at downwind edge of source area:

$$C = q\left[\int_{50}^{t_L} \frac{2}{\sqrt{2\pi}\,\sigma_z}\,dt + \int_{t_L}^{t_s} \frac{1}{L}\,dt\right]$$

where $t_s = \frac{S}{u} =$ time required to travel across the source area with the mean wind speed, sec

B. Average of city area:

$$C = \frac{uq}{S}\int_{50}^{t_L}\int_{50}^{t_L} \frac{2}{\sqrt{2\pi}\,\sigma_z}\,dt\,dt + \int_{t_L}^{t_s}\int_{t_L}^{t_s} \frac{1}{L}\,dt\,dt$$

IV. Meteorological Parameters:

Meteorological parameters required in the above model are mean wind speed and mixing layer height. The diffusion parameters are taken from Turner's (1964) time-oriented interpretation of the Pasquill diffusion parameters. Class C was used for afternoons and Class D for mornings. The afternoon mixing layer ceiling was defined to be the height above the surface at which a dry adiabatic lapse rate from the maximum surface temperature intersected the morning radiosonde temperature sounding. The morning mixing layer ceiling was defined to be the height at which a dry adiabatic lapse rate from a surface temperature of 5° C greater than the morning minimum intersects the morning radiosonde temperature sounding.

V. Validation Results:

Pollutant	Location	Time Of Day	Observing Period	No. of Periods	No. of Stations	Range of Observations pphm	Number of Comparisons Within ± 2 pphm	Regression of Observed On Calculated, pphm		
								Correlation Coefficient	Intercept	Slope
NO_x	Los Angeles	1500-1700	1963	36	7 to 9	4.5 to 23.5	30 of 36	0.88	0.06	1.02
SO_2	Nashville	1200-1400	Oct - Mar 1958-59	31	7	0 to 4.2	90% within ± 1 pphm	0.84	0.25	1.16
NO_x	Washington (a)	1300-1700	1962-64	58	1	1 to 17	(b)	0.83	0.77	0.92
NO_x	Los Angeles	0700-0900	1963	35	7 to 9	5 to 56	51% within 5 pphm of regression line	0.80	5.23	0.58
SO_2	Nashville	0400-0600	Oct - Mar 1958-59	31	7	0 to 9.8	All within 3 pphm of regression line	0.84	1.77	0.41

(a) Calculated concentrations are for downwind edge of city.
(b) Not reported.

Exhibit A-7. Model Implementation by Koogler, Sholtes, Davis and Harding (1967)

I. Scope:

Estimate continuous or 24-hour mean ground-level concentrations from multiple sources in an urban area.

II. Treatment of Sources:

Sources with an emission rate greater than 10^4 g/hr are treated as point sources. All other sources are treated as an area source. Estimate plume rise (ΔH) using the Holland formula (i.e., use stack diameter, gas velocity and gas heat content; see Slade 1968). The effective source height is:

$$h = (H + \Delta H) \left(\frac{x}{2000}\right)^{\frac{2}{3}}$$

If an inversion base exists aloft, h equals the height of the inversion base. If an inversion exists at ground level and an adiabatic lapse rate exists above 1.25 times H, no ground-level concentrations are calculated. Divide the area source into square mile subdivisions. Each square is treated as a uniform crosswind line source 1609m long.

III. Computational Equations

Divide 24-hour interval into periods of constant meteorological conditions (i.e., wind direction, wind speed and stability classification) and duration t_k.

A) For point sources such that $x < ut_k$

$$C_p = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left\{-0.693 \frac{t}{t_{50}} - \frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2 - \frac{1}{2}\left(\frac{h}{\sigma_z}\right)^2\right\}$$

B) For finite line sources such that $x < ut_k$

$$C_A = \frac{Q}{1609\sqrt{2\pi}u\sigma_y\sigma_z} \text{esp}\left(-0.693 \frac{t}{t_{50}}\right) \cdot \left[\text{erf}\left(\frac{804.5 - y}{\sqrt{2}\,\sigma_y}\right) + \text{erf}\left(\frac{804.5 + y}{\sqrt{2}\,\sigma_y}\right)\right]$$

Contributions due to emissions during one preceding period are also used as follows:

C) When the wind direction is unchanged from the preceding period, apply the above equations to sources with an alongwind distance from source to receptor such that $u_2t_k \leq x < (u_1 + u_2)t_k$ where u_1 is the wind speed of the preceding period and u_2 is the wind speed of the current period.

D) When the wind direction differs from the preceding period, the plume from each source during the preceding period is treated as a line source. The concentration distribution along the new line source is the crosswind integral of the ground-level concentration. The line source is allowed to diffuse in the new wind direction allowing only vertical dispersion and decay effects.

The total concentration at a point during a period is the sum of all point, finite line, and preceding period emissions. The concentration for a 24-hour period is the average concentration over all subdivisions of the period.

IV. Meteorological and Other Non-Source Parameters:

For each period of constant meteorological conditions, determine the wind direction, wind speed and stability classification. The wind speed is treated as constant to 65m. Above 65m the relation of wind speed (u_1) at height (z_1) to the wind speed (u_2) at height (z_2) is:

$$u_1 = u_2\left(\frac{z_1}{z_2}\right)^{\frac{n}{2-n}}$$

where n is a stability oriented parameter varying from 0.18 for extremely unstable conditions to 0.51 for stable conditions. Estimate stability classifications defined by Gifford (1961) from vertical temperature measurements. Estimate diffusion parameter values for σ_y and σ_z for each stability classification from Gifford's presentation (1961). Use 4 hours for the half-life (t_{50}) of SO_2.

V. Validation Results:

Calculated and observed 24-hour average SO_2 concentrations were compared for 11 sampling stations. Data were obtained for 12 days during December 1965 and January 1966 and resulted in 111 comparisons. The observed values ranged from 0 to 3 pphm. When values are categorized to the nearest 0.5 pphm, a chi square test of significance on a two-way contingency table (observed versus predicted) showed the calculated prediction was significant at the 0.1% level. Furthermore, 95% of the computed concentrations were within ±1 pphm of the observed concentrations.

Exhibit A-8. Model Implementation by Martin and Tikvart (1968) (also Martin 1971)

I. Scope:

Average seasonal concentrations of pollutants at multiple receptors from multiple sources.

II. Treatment of Sources:

Treat sources with emission rates greater than 100 tons/year as elevated point sources. Estimate plume rise from the Holland equation with a stability oriented correction factor (e.g., see TRW Systems Group 1969). Treat all other sources as an area source. Subdivide the area source into squares of 1 to 10 km on a side and determine the rate of emission and average effective height h. Each area source square is treated as a virtual point which emits at a rate equal to the emission rate of the total square at a distance (r_o) upwind of the center of the square dependent on the size of the area, i.e.:

$$r_o = \frac{\sqrt{A}}{0.393}$$

III. Computational Equations:

Both the area source and large point sources are represented by a set of point sources. All wind directions in a 22.5° sector centered on a 16-point compass azimuth are assumed to occur with equal probability. The emission rate is assumed to be constant or at least independent of meteorological conditions. Beyond a distance of 2 r_m the vertical distribution of pollutants is uniform due to the influence of the mixing layer ceiling, where r_m is the travel distance such that $\sigma_z(r_m) = 0.47\ L_k$. In terms of the joint frequency distribution of meteorological parameter classes, the concentration at a receptor point from all sources is given as follows:

For $r \leq r_m$

$$\overline{C}\,(r) = \sum_{i=1}^{N} \sum_{j=1}^{6} \sum_{k=1}^{5} f(D_i,\, u_j,\, s_k) \frac{2Q_i}{\sqrt{2\pi}\, \sigma_z(r_i,\, s_k)\, u_j\left(\frac{2\pi r_i}{16}\right)}$$

$$\cdot\ \exp\left\{-\frac{1}{2}\left[\frac{h_i}{\sigma_z(r_i,\, s_k)}\right]^2\right\}$$

For $r \geq 2r_m$

$$\overline{C}\,(r) = \sum_{i=1}^{N} \sum_{j=1}^{6} \sum_{k=1}^{5} f(D_i,\, u_j,\, s_k) \frac{Q_i}{\left(L_k u_j \frac{2\pi r_i}{16}\right)}$$

For $r_m < r < 2r_m$

$$\overline{C}\,(r) = \overline{C}\,(r_m) + \frac{r - r_m}{r_m}\left[\overline{C}(2r_m) - \overline{C}(r_m)\right]$$

In the above equations:

N = number of point sources (total of large and virtual points)

D_i = wind direction class for azimuth from receptor to ith source

s_k = k th stability class

$\sigma_z(r_i,\, s_k) = \left[(a r_i^{\,b} + c)^2 + \sigma_h^{\,2}\right]^{0.5}$

r_i = distance from receptor to ith source (note that virtual point sources are displaced a distance r_o upwind of the center of the area source square)

a, b, c = empirical diffusion parameters dependent on s_k and r_i

σ_h = initial vertical dimension of plume

IV. Meteorological Parameters:

Use hourly meteorological observations to determine the joint frequency distribution of meteorological conditions consisting of 480 combinations of 16 wind direction classes, 5 stability classes (based on Turner's 1964 definitions) and 6 wind speed classes.

Use the Pasquill diffusion parameters for σ_z expressed as mathematical equations of the form $\sigma_z = ax^b + c$ where the parameters a, b and c are defined separately for each stability class and various ranges of x. The mixing layer ceiling is taken as a function of the stability class and the climatological afternoon mixing layer height (L_c), varying from 100m for class 5 to 1.5 L_c for class 1.

V. Validation Results:

Mean winter concentrations were calculated for 40 St.Louis stations. A regression analysis of observed values on calculated values was performed for the 40 locations. The regression analysis was repeated with 5 stations which were strongly influenced by point sources omitted. The results were:

	40 Stations	35 Stations
Correlation coefficient	0.60	0.84
Slope of regression line	0.266	0.56
Intercept of regression line	0.026	0.011

Exhibit A-9. Model Implementation by Fortak (1970)

I. Scope:

Estimate long-term concentrations of ground-level SO_2 concentrations from multiple sources and derive the associated frequency distribution of short-term concentrations.

II. Treatment of Sources:

Treat sources with an emission rate greater than 1 kg/hr as point sources. Estimate the plume rise using Stumke's empirical formula which is similar to the CONCAWE formula (e.g., see Briggs 1969). Treat small industrial sources and emissions during space heating by dwellings as an area source. Estimate the seasonal emission rate (Q_A) for each 500m by 500m square of the area source. Use an emission height of 25m for squares in a downtown area and 15m for squares in a suburban area. A simple, but unspecified, procedure is used to estimate the effective height of an area source. Represent each square by a set of n by n indentical point sources, equally spaced over the square. Each point has an emission rate of Q_A/n^2. Values of n^2 from 81 to 144 are recommended.

III. Computational Equations:

Consider a fixed retangular horizontal coordinate with ξ-axis pointing east and η-axis pointing north. For wind direction θ, measured from north in radians, the alongwind distance x_i and crosswind distance y_i between a point source at location (ξ_i, η_i) and a receptor at location (ξ_R, η_R) are:

$$x_i = (\xi_R - \xi_i) \cos (\frac{3}{2}\pi - \theta) + (\eta_R - \eta_i) \sin (\frac{3}{2}\pi - \theta)$$

$$y_i = (\eta_R - \eta_i) \cos (\frac{3}{2}\pi - \theta) - (\xi_R - \xi_i) \sin (\frac{3}{2}\pi - \theta)$$

The concentration at a receptor from all point sources (including area source representations) during a specific combination of meteorological conditions is:

$$C = \frac{1}{2\sqrt{2\pi}\, L} \sum_{i=1}^{N} \frac{Q_i}{u_1(H_i,\ s_k)\ \sigma_y\ (x_i,\ s_k)} \exp\left\{-0.693\frac{t_i}{t_{50}} - \frac{1}{2}\left[\frac{y_i}{\sigma_y(x_i,\ s_k)}\right]^2\right\}$$

$$\cdot\left[\Theta_3\left(\frac{h_i - z_r}{2L},\ \frac{\sigma_z{}^2(x_i,\ s_k)}{2L^2}\right) + \Theta_3\left(\frac{h_i + 3_R}{2L},\ \frac{\sigma_z{}^2(x_i,\ s_k)}{2L^2}\right)\right]$$

where $\Theta_3(v,\ w) = \frac{1}{\sqrt{\pi w}} \sum_{i=-\infty}^{\infty} \exp\left\{-\ \frac{(v + i)^2}{w}\right\}$

The concentrations associated with each possible combination of the classes of the three meteorological parameters which have a non-zero frequency of occurrence may be calculated and ordered from low to high. Summing the frequency of occurrence associated with ordered concentrations a frequency distribution of expected concentrations at a point may be constructed. From the constructed frequency distribution the concentration for any probability level may be estimated. The frequencies of occurrence may also be used to calculate the long-term mean or the mean for any particular wind direction class.

IV. Meteorological and Other Parameters:

Determine the joint frequency distribution of meteorological parameters including wind direction, wind speed and stability class for the long-term period of interest (e.g., month, seasonal, heating period). Use 36 wind direction classes, 7 wind speeds and the 5 stability classes of Turner (see text, Tables 2 and 3) to define the meteorological conditions. For low-level emissions (i.e., area sources) use the Pasquill diffusion parameters for σ_y and σ_z (e.g., see text, Figures 2 and 3). For high-level emissions (i.e., large point sources) use a slightly modified version of the Brookhaven diffusion parameters presented by Fortak (see Stern 1970). Treat the power-law used to extrapolate observed wind speed class values to values at various stack heights as a function of atmospheric stability using values reported in the literature. Use 500m for the height of the mixing layer ceiling (L).

V. Validation Results:

Calculated and observed SO_2 concentrations were compared at 4 locations in Bremmen, Germany, for the 1967-68 heating season (i.e., November through May). The cumulative frequency distributions of calculated and observed concentrations for the season were compared graphically at each location. In general, the observations were overestimated at three stations and underestimated at one. Monthly and seasonal means for the four locations were also compared. The observed seasonal means were 0.06 mg/m^3 at one station and 0.08 mg/m^3 at the other three. The calculated minus observed seasonal concentrations were -0.04, 0.01, 0.02 and 0.04 mg/m^3. The observed monthly means (for 4 stations times 7 months) ranged from 0.03 to 0.13 mg/m^3. The calculated minus observed monthly concentrations for the 28 values ranged from -0.05 to 0.06 mg/m^3.

Exhibit A-10. Model Implementation by Milford, McCoyd, Aronowitz and Scanlon (1970)

I. Scope:

Use short-term pollutant concentration estimates to give long-term concentrations.

II. Treatment of Sources:

Treat electric power plants as point sources. Determine the emission rate and effective height of each plant. Treat other sources as an area source. Area source characteristics are available from emission inventory surveys by square subdivisions. Combine characteristics in the outer regions of the source area to define characteristics in terms of coarser subdivisions. Represent each square by treating it as a double virtual point, i.e., as a two-dimensional plume with assumed vertical and horizontal diffusion parameter values at the center of the square. Determine the emission rate, initial vertical and horizontal diffusion parameter value, and mean effective source height for each subdivision.

III. Computational Equations:

Since both the area source and point source are treated as a set of point sources the standard Gaussian plume equation is applicable to each calculation. Use a version (specific equation not specified) which includes wind speed, wind direction, stability class, mixing ceiling, source location relative to a receptor, source emission rate and source effective height as parameters. Parameter values are fixed for a short-term period. With an inversion aloft, assume no effect due to the inversion up to a certain distance. At some greater distance assume uniform vertical mixing. Use linear interpolation at intermediate distances.

IV. Meteorological Parameters:

Make estimates of the wind direction, the wind speed and the mixing layer ceiling representative of the region for a selected period. Estimate a stability class appropriate for use with the McElroy-Pooler (1968) diffusion parameters. For use with virtual point sources it is necessary to determine a virtual distance associated with the assumed initial diffusion parameter. Determine diffusion parameters for each downwind travel distance from source to receptor by determining the diffusion value corresponding to a distance equal to the sum of the virtual distance plus the travel distance.

V. Validation Results:

Comparisons were made between calculated and observed SO_2 concentrations at 10 telemetry stations in New York City for the July through August 1969 period. Calculations were made for each hour of the period using wind speed and direction data from La Guardia Airport, an infinite mixing layer ceiling, plume rise estimates for large point sources based on a 10 mph wind speed using the CONCAWE formula (e.g., see Briggs 1969), and the McElroy-Pooler stability class 4 (see text, Table 5) diffusion parameters. The means of all calculated concentrations for all hours and all stations were 6.8 and 6.6 pphm for July and August, respectively. The corresponding observed means were 7.0 and 7.5 pphm. Of the 20 sets of individual station monthly means, 15 calculated means were within a factor of 2 of observed means. The largest discrepancy was an overprediction by a factor of 4. A summary of statistics reported for comparisons of hourly comparisons is as follows:

	July 1969		August 1969	
	Mean Rel. Error	Std. Dev. of Rel. Error	Mean Rel. Error	Std. Dev. of Rel. Error
Comparisons of all station means	-0.36	2.3	-0.58	2.8
Range of comparisons at individual stations	-3.4 to 0.42	0.66 to 5.1	-4.3 to 0.52	0.69 to 6.0

Exhibit A-11. Model Implementation by Ludwig, Johnson, Moon and Mancuso (1970)

I. Scope:

Calculate short-term (single steady state) carbon monoxide (CO) concentrations in urban areas for producing (1) concentration isopleths for a specific time, (2) concentration histories for a specific location and (3) long-term climatological summaries of concentrations for specific locations.

II. Treatment of Sources:

Treat all CO emissions as a ground-level area source. For each receptor location considered, estimate the emission rate per unit area applicable to angular segments centered on a line pointing upwind from the receptor. The angular segments have a width of 45° out to 1 km. Beyond 1 km the angular segments have a width of 22.5°. The segments are bounded by arcs with radii of 0.125, 0.25, 0.5, 1, 2, 4, 8 and 16 km.

III. Computational Equations:

Use the Gaussian plume diffusion model for treating emissions over travel distances which are less than the distance (r_T) at which the Gaussian plume model concentration equals that obtained from uniform mixing beneath the mixing layer ceiling.

$$r_T = \left(\frac{0.8L}{a_{ij}}\right)^{b_{ij}} \qquad \text{where } r_N < r_T < r_{N+1}$$

Beyond this distance uniform vertical mixing is assumed. The resultant concentration at a receptor from eight sectors is:

$$C = \frac{1}{u}\left\{0.8\left[\sum_{i=1}^{N-1} Q_i \frac{r_{i+1}^{1-b_{ij}} - r_i^{1-b_{ij}}}{a_{ij}(1 - b_{ij})}\right] + Q_N\left[\frac{0.8\left(r_T^{1-b_{Nj}} - r_N^{1-b_{Nj}}\right)}{a_{Nj}(1 - b_{Nj})} - \frac{r_{N+1} - r_T}{L}\right] + \frac{1}{L}\sum_{i=N+1}^{8} Q_i(r_{i+1} - r_i)\right\}$$

IV. Meteorological Parameters:

Estimate wind direction, wind speed, mixing layer ceiling, and stability class. Use wind direction and speed observations from airport weather stations. Estimate mixing layer ceilings using the nearest 1200Z radiosonde data and the maximum afternoon temperature (T_a) by the following values:

Time of Day	L
Midnight to 1200 GMT	L_m
1200 GMT to 1400 LST	L_1
1400 LST to Midnight	L_2

$$L_m = 29.3\left(\frac{T_m + T_s}{2}\right)\phi\left[\frac{0.298\left(\frac{T_m - T_s}{p_m - p_s}\right) - 0.0633}{\frac{p_m + p_s}{2}\left(\frac{T_m - T_s}{p_m - p_s}\right) - 0.287\left(\frac{T_m + T_s}{2}\right)}\right]$$

$$L_1 = \left(\frac{T - T_m}{T_a - T_m}\right)(L_a - L_m) + L_m$$

$$L_a = 29.3\left(\frac{T_x + T_a}{2}\right)\ln\frac{p_a}{p_x}$$

$$L_2 = \left(\frac{H - 14}{10}\right)(L_n - L_a) + L_a$$

where T_m = surface temperature in 1200Z radiosonde

p_m = surface pressure in 1200Z radiosonde

T_s = temperature of first significant level in 1200Z radiosonde

p_s = pressure of first significant level in 1200Z radiosonde
ϕ = population of the urban area
T_a = maximum afternoon surface temperature
p_a = surface pressure corresponding to T_a
p_x = pressure in the 1200Z radiosonde corresponding to a potential temperature given by T_a and p_a
T_x = temperature in the 1200Z radiosonde corresponding to p_x
H = hour of interest
L_n = L_m for 1200Z radiosonde of following day

Determine which of five Pasquill stability classes is appropriate from the solar elevation angle (α), the fraction of sky covered by clouds (N), and the wind speed using the following table:

Wind Speed (Knots	$0<I\leq 0.33$	$0.33<I\leq 0.67$	$0.67<I$	$\alpha\leq 0$	
				$0.5\leq N$	$N\leq 0.4$
≤ 3	A	B	B	E	E
3-6	A	B	C	D	E
6-10	B	C	C	D	D
10-12	C	C	D	D	D
≥ 13	C	D	D	D	D

$$I = (1 - 0.5N)\sin\alpha$$

$$\alpha = \arcsin\left\{\sin\left[\mathrm{arctam}\left(-\tan 23.5^\circ \cos\left[\frac{2\pi(d+10)}{365}\right]\right)\right]\sin\Psi + \cos\left(\frac{12-H}{2\pi}\right)\cos\Psi\cdot\cos\left[\arctan\left(-\tan 23.5^\circ\cos\left[\frac{2\pi(d+10)}{365}\right]\right)\right]\right\}$$

The diffusion parameters a_{ij} and b_{ij} are related to the Pasquill σ_z diffusion parameter (see text, Figure 2) for each stability class j defined in the above table by fitting a simple relationship to the curves presented by Gifford (1961), over travel distances for the ith source segment, i.e.:

$$\sigma_z = a_{ij}\, x^{b_{ij}} \qquad \text{for } r_i < x \leq r_{i+1}$$

For the source segment closest to the receptor:

$$b_{ij} = 0$$

$$a_{ij} = \sigma_z \text{ for class } j \text{ at } x = 125\text{m}$$

For other parameter values, see author's text (Ludwig, et al. 1970).

V. Validation Results:

Comparisons were made between calculated and observed hourly concentrations of CO during weekdays of March to December 1964 for the St. Louis CAMP station. The correlation coefficients ranged from 0.16 to 0.45 with a mean of 0.31. The RMSE ranged from 4.7 to 8.8 ppm with a mean of 6.2 ppm. A good portion of the RMSE is attributable to a background level which was estimated for each month and found to vary between 3.5 and 7.0 ppm.

Exhibit A-12. Model Implementation by Calder (1970)

I. Scope:

Estimate long-term average concentrations of gaseous pollutants using point and area source emission inventory data together with climatological frequency data for wind speed, wind direction, atmospheric stability and mixing depth.

II. Treatment of Sources:

Treat large sources with emission rates in excess of 100 tons/yr as elevated point sources. Determine the seasonal emission rate, physical stack height, and additional stack parameters required to estimate plume rise (e.g., see Briggs 1969). Treat other emissions as an area source. Determine seasonal emission rates for sub-areas of the area source which are chosen in relation to the spatial uniformity of the source distribution. Determine the uniform effective height which is most applicable for the area source (e.g., 20m was selected for St. Louis).

III. Computational Equations:

The total average concentration at a receptor due to both point and area sources is $\overline{C} = C_A + C_p$ where:

$$C_p = \frac{16}{2\pi} \sum_{i=1}^{N} \sum_{j} \sum_{k} \frac{Q_i \; f\,(\theta_i, j, k)\; S\,(x_i, z_r; u_j, k)}{x_i}$$

where

j = wind speed class

k = Pasquill stability class as defined by Turner (see Tables 2 and 3)

z_r = height of receptor location

The form of the factor S $(x_i, z_r; u_j, k)$ is dependent on the degree to which the mixing layer ceiling (L_k) restrains vertical mixing as follows:

For $\sigma_z(x_i; k) \leq \frac{L_k}{2.15}$,

$$S(x_i, z_r; \mu_j, k) = \frac{1}{\sqrt{2\pi}\, u_j\, \sigma_z(x_i; k)} \left[\exp\left\{- \frac{(z_r - H_i - \Delta H_i)^2}{2\sigma_z{}^2(x_i; k)}\right\} + \exp\left\{- \frac{(z_r + H_i + \Delta H_i)^2}{2\sigma_z{}^2(x_i; k)}\right\}\right]$$

For $\sigma_z(x_i; k) \geq \frac{2L_k}{2.15}$,

$$S(x_i, z_r; \mu_j, k) = \frac{1}{u_j\, L_k}$$

For $\frac{L_k}{2.15} < \sigma_z(x_i; k) < \frac{2L_k}{2.15}$, use linear interpolation between the two forms.

$$C_A = \frac{16}{2\pi} \int_0^\infty \left\{\sum_{i=1}^{16} q_i(x) \sum_j \sum_k f(i, j, k)\, S(x, z_r; u_j, k)\right\} dx$$

$$\text{where } q_i\,(x) = \int_{\theta_i}^{\theta_{i+1}} Q(x, \theta)\, d\theta \quad (\theta_{17} = \theta_1)$$

Apply the trapezoid rule to numerically integrate the equations. The θ_i values are 22.5° apart. The $q_i(x)$ integral may be evaluated using 2.25° increments for θ. The C_A integral may be evaluated using 100m increments from the receptor to the edge of the source area.

IV. Meteorological and Diffusion Parameters:

The meteorological parameters in the above model are wind speed, wind direction, stability classification, and climatological mixing layer ceiling (e.g., as tabulated by Holzworth, 1964). Generate the joint frequency distribution of wind speed, wind direction, and stability classification using standard Weather Bureau airport observations. On this basis, there are 16 wind direction categories with dividing azimuths θ_i, 6 wind speed categories (each with a representative value u_j), and 5 stability categories corresponding to the A to E Pasquill diffusion parameter classes, but determined using Turner's criteria (see text, Figures 2 and 3). The mixing layer ceiling L_k is determined from the seasonal average daily maximum mixing depth (L in Meters) and the stability classification as follows:

Stability Classification	L_k (meters)
A	1.5 L
B, C, D (day)	L
D (night)	0.5 (100 + L)
E	100

The Pasquill diffusion parameters $\sigma_z(x; k)$ are determined from the following relationships fitted to curves presented by Gifford (1961).

$$\sigma_z(x; k) = a_{ki}\, x^{b_{ki}} + c_{ki}$$

For each value of k there are three possible sets of coefficients (a_{ki}, b_{ki}, c_{ki}). The proper set depends on which of 3 distance ranges contains x (i.e., <100, 100-1000, >1000; see Calder (1970) for the 45 coefficient values).

V. Validation Results:

Calculated and observed seasonal mean SO_2 concentrations were compared for St. Louis winter season data (Dec. 1, 1964 to Feb. 28, 1965). A regression analysis of observed on calculated values ($\mu g/m^3$) for 40 sampling stations resulted in a correlation coefficient of 0.775 an intercept of 19.98 and a slope of 0.26.

Exhibit A-13. Model Implementation by Singer and Smith (1970, 1966)

I. Scope:

Estimate short-term concentrations from multiple single sources for stable pollutants.

II. Treatment of Sources:

Identify the pollutant emission rate, geographical location, stack height and stack and emission characteristics related to plume rise for each source. Treat each emission as a continuous point source.

III. Computational Equations:

The concentration at each receptor point is the sum of contributions from each of N sources.

$$C = \sum_{i=1}^{N} \frac{Q_i}{(\sigma_y)_i (\sigma_z)_i u_i} \exp \left\{ - \frac{(H_i + \Delta H_i)^2}{2(\sigma_z)_i^{\,2}} + \frac{y_i^{\,2}}{2(\sigma_y)_i^{\,2}} \right\}$$

IV. Meteorological and Diffusion Parameters:

The wind speed is assumed to be horizontally uniform but varies with height as a power function in which the power (q) is given by the atmospheric stability. In order to account for the effect of the wind profile on the growing vertical dimension of the plume from a point source, a "mean equivalent wind speed" is defined. The height in the wind profile at which the "mean equivalent wind speed" occurs was found to be $\hat{z} = 0.62\sigma_z$.

For $H_i + \Delta H_i \leq 0.62(\sigma_z)_i$

$$u = \delta(H_i + \Delta H_i)^q$$

For $H_i + \Delta H_i > 0.62(\sigma_z)_i$

$$u = \delta\left[0.62(\sigma_z)_i\right]^q$$

δ may be estimated from a wind speed u_a at height z_a, $\delta = \frac{u_a}{{z_a}^q}$

q varies from 0.15 for unstable conditions to 0.50 for stable conditions.

The diffusion parameters are given in terms of distance x_i and Brookhaven gustiness classes (Singer and Smith 1966).

$$(\sigma_y)_i = a_k \, x_i^{p_k}$$

$$(\sigma_z)_i = b_k \, x_i^{p_k}$$

There is a set of a_k, b_k and p_k values specified for each of the 4 Brookhaven gustiness classes as follows:

Brookhaven Gustiness Class	a_k	b_k	p_k
B_2	0.40	0.41	0.91
B_1	0.36	0.33	0.86
C	0.32	0.22	0.78
D	0.31	0.06	0.71

$(\sigma_z)_i$ is further limited by the mixing layer ceiling restriction that $(\sigma_z)_i \leq \frac{L}{1.25}$.

V. Validation Results:

Calculated and observed 6-hour mean SO_2 concentrations were compared. The data was selected from 20 sources, 5 SO_2 sampling locations, Weather Bureau airport observations, supplementing wind data and aircraft observations. The mean observed and calculated concentrations for all 6-hour periods at each location were:

Station	Mean Observed	Mean Calculated	Number of Comparisons
Ferry	.049	.043	31
Whitney	.029	.014	47
Count	.035	.008	31
Temple	.075	.024	8
Fairhaven	.048	.033	8

Section 1.0

INTRODUCTION

This appendix summarizes the St. Louis data which have been obtained and identifies their sources.

Punched cards were received from the government (Division of Meteorology, National Environmental Research Center, Research Triangle Park, EPA) which contain emission information, meteorological observations, air quality observations, and algorithms for estimating SO_2 emission rates for St. Louis. The data covered the period 1400 December 1, 1964 to 1400 February 28, 1965. The characteristics and sources of these data are briefly reviewed below.

Section 2.0

EMISSION DATA

Turner (1968b) has developed an algorithm for estimating SO_2 emissions as a function of location, temperature, time of day and day of week. This algorithm represents emissions in terms of two types of sources, point sources and area sources. The computation formulas are presented below for each type of source both in terms of the input provided by the punch cards and in terms of the original information which is the basis for the punched card data. Much of the original information is not available; however, formulations in terms of original data help to indicate the nature of input errors and uncertainties associated with the data and the derived emission estimates.

2.1 POINT SOURCES

Information regarding utility power plants and industrial plants are available in different levels of detail. As a result, each is discussed separately.

2.1.1 Industrial Sources

Industrial SO_2 emissions are the sum of emissions from process and space heating fuel consumption. The emissions from process fuel requirements are estimated by multiplying a peak process emission rate by utilization factors related to the day of the week and the hour of the day. The emissions from space heating requirements are determined in terms of the outside air temperature deficit from 65°F. The algorithm used for St. Louis is:

$$Q(t) = Q_p \, F_d(t) \, F_h(t) + q_x \, D_c(t) \tag{1}$$

where

$Q(t)$ = SO_2 emission rate

Q_p = peak process SO_2 emission rate

$F_d(t)$ = fraction of peak for day of week

$F_h(t)$ = fraction of peak for hour of day

q_x = heating fuel SO_2 emission rate per degree (i.e., per degree of ambient air temperature below 65°F)

$D_c(t) = 65 - [T(t) + \Delta_c(t)]$

$T(t)$ = ambient air temperature, °F

$\Delta_c(t)$= commerical correction factor, °F (Turner 1968a).

The quantities Q_p, $F_d(T)$ and $F_h(t)$ were obtained by Turner from survey questionnaires submitted by plant operators. The quantity q_x may be obtained from annual emission information by the following formulae:

$$q_x = \frac{1}{D_a} \sum_{j=1}^{n} W_j \, S_j \tag{2}$$

q_x = SO_2 emission rate per degree

W_j = annual quantity of fuel j used (from survey)

S_j = sulfur dioxide emitted per unit fuel i (from survey)

D_a = annual number of degree days

or

$$q_x = \frac{1}{D_w} \sum_{j=1}^{n} (F_w)_j \, W_j \, S_j \tag{3}$$

q_x = SO_2 emission rate per degree

$(F_w)_j$ = fraction of annual quantity of fuel j used in winter season

D_w = winter season degree days.

In terms of initial source data:

$$Q(t) = Q_p F_d(t) F_h(t) + [65 - T(t) - \Delta_c(t)] \frac{1}{D_a} \sum_{j=1}^{n} W_j S_j \qquad (4)$$

In addition to the emission rate parameters, i.e., Q_p, F_d, F_h, q_x and Δ_c, the furnished punched card data included location coordinates of the source, the physical height of the source stack (effective height if no plume rise data is given) and the plume-rise, wind-speed product. The plume-rise, wind-speed product was estimated by means of Holland's (1953) formula using data obtained in the course of an inventory survey. Only the resultant product data were available for this study.

2.1.2 Power Plant Sources

Power plant SO_2 emissions were estimated by two different methods, each developed to fit a certain type of available data. For four plants, stack operating characteristics were obtained as a function of plant output. For these plants hourly outputs in megawatts were available for the entire data period. For one plant this information was broken down by generating unit. The information included graphs of fuel weight flow rate, stack temperature and stack exit gas volume flow rate as functions of power output. The fuel flow rates were found to be appropriately represented by a linear relationship of the form

$$F = A_1 + A_2 L \tag{5}$$

where F = fuel weight flow rate, lb/min

L = power output, megawatts

A_1, A_2 = empirical parameters.

The stack temperature and volume flow rate were also estimated by a linear relationship with power output. However, it was found necessary to divide the range of power outputs from zero to a peak value into 3 equal parts and to use a linear approximation over each part or class of the range. Two values of stack temperature and of stack gas flow rate were selected to define the end points of a linear approximation for each class of power output values. However, a single end point was selected for adjacent classes. As a result, four values of stack temperature and flow rate and the peak power output allow one to construct a linear approximation of these parameters as a function of power output. Specifically,

$$T_s = T_\ell + \frac{L - L_\ell}{L_p/3} (T_u - T_\ell) \tag{6}$$

where T_s = stack temperature, °F

L = power output, mw

L_ℓ = lower limit of power output class (i.e., $L_\ell = 0, \frac{1}{3} L_p$ or $\frac{2}{3} L_p$)

L_p = peak power output, mw

T_ℓ = stack temperature for power load of L_ℓ, °F

T_u = stack temperature for power load of $L_\ell + \frac{1}{3} L_p$ (upper limit of class), °F.

Similarly, the stack volume flow rate for power output L lying in the power output class with lower limit L_ℓ is

$$V_s = V_\ell + \frac{L - L_\ell}{L_p/3} (V_u - V_\ell) \tag{7}$$

where V_s = stack gas volume flow rate, 10^6 ft^3/min

V_ℓ = stack gas volume flow rate for power load of L_ℓ, 10^6 ft^3/min

V_u = stack gas volume flow rate for power load of $L_\ell + \frac{1}{3} L_p$, 10^6 ft^3/min.

Values of the class limits and the peak power load for seven emission points in the St. Louis area are given in Table B-1. Values of the empirical parameters for estimating fuel weight flow rate are also shown. The fuel flow rate may be converted to an SO_2 emission rate by means of a proper SO_2 emission factor and the sulfur content of the fuel as follows:

$$Q = F\ E\ (\frac{S}{100}) \tag{8}$$

where Q = SO_2 emission rate, lb/min

F = fuel weight flow rate, lb/min

E = SO_2 emission factor, lb SO_2/lb S (~ 2)

S = sulfur content of fuel, percent.

T_ℓ = stack temperature for power load of L_ℓ, °F

T_u = stack temperature for power load of $L_\ell + \frac{1}{3} L_p$ (upper limit of class), °F.

Similarly, the stack volume flow rate for power output L lying in the power output class with lower limit L_ℓ is

$$V_s = V_\ell + \frac{L - L_\ell}{L_p/3} (V_u - V_\ell) \qquad (7)$$

where V_s = stack gas volume flow rate, 10^6 ft^3/min

V_ℓ = stack gas volume flow rate for power load of L_ℓ, 10^6 ft^3/min

V_u = stack gas volume flow rate for power load of $L_\ell + \frac{1}{3} L_p$, 10^6 ft^3/min.

Values of the class limits and the peak power load for seven emission points in the St. Louis area are given in Table B-1. Values of the empirical parameters for estimating fuel weight flow rate are also shown. The fuel flow rate may be converted to an SO_2 emission rate by means of a proper SO_2 emission factor and the sulfur content of the fuel as follows:

$$Q = F\,E\,(\frac{S}{100}) \qquad (8)$$

where Q = SO_2 emission rate, lb/min

F = fuel weight flow rate, lb/min

E = SO_2 emission factor, lb SO_2/lb S (~ 2)

S = sulfur content of fuel, percent.

Table B-1. Stack Emission Parameters for St. Louis Power Plants (1964-65)

Plant	Unit Number	Coefficient of Fuel Flow Rate (F, lb/min) $F=A_1+A_2L$ L=Power output, mw		Peak Fuel Flow Rate, lb/min	Stack Temperature Class Limits, °F				Stack Flow Rate Class Limits, 10^6 ft^3/min			
		A_1	A_2	L_p	T_1	T_2	T_3	T_4	V_1	V_2	V_3	V_4
Meramec	1 and 2	50	10.89	150	281	294	312	343	40	170	320	500
Meramec	3	100	10.43	300	242	262	290	336	210	375	625	1015
Meramec	4	100	10.75	405	236	267	323	372	260	490	840	1460
Venice		20	13.0	480	252	293	312	352	30	625	1180	1840
Cahokia		0	16.67	150	350	406	420	434	20	260	520	835
Ashley		0	1.536	1500	296	323	342	356	5	225	440	665

For another power plant site, an average emission rate was estimated for each two-hour period of the day for each of four emission sites. A corresponding estimate of the wind speed, plume rise product was also made for each site. These estimates were assumed to be representative of all days in the data period. The estimates were derived by government personnel based on discussions with the plant operator. The estimates were part of the set of punched card data furnished by the government.

In addition to the emission data described above, the government furnished punched card data included location coordinates and physical stack heights.

2.2 AREA SOURCES

Area source emissions for SO_2 were available for St. Louis in 5000 ft by 5000 ft grid squares. Emission data for several categories of sources (including residential, commercial, river vessels, automobiles, railroads, backyard burning and industrial) were available on punched cards for each grid square. The information amounted to a parameter estimate for use in the following algorithm developed by Turner (1968b):

$$\begin{aligned} Q(t) = {} & Q_r + q_r D_r(t) + Q_c F_c(t) + q_c D_c(t) + Q_v + Q_a F_a(t) \\ & + Q_w + Q_b + q_x D_c(t) + Q_p F_d(t) F_h(t) \end{aligned} \qquad (9)$$

$$D_r(t) = 65 - T(t) - \Delta_r(t)$$

$$D_c(t) = 65 - T(t) - \Delta_c(t)$$

where $Q(t)$ = SO_2 emission rate

Q_r = base residential SO_2 emission rate

q_r = residential heating SO_2 emission rate per degree

$T(t)$ = ambient air temperature

$\Delta_r(t)$ = residential correction factor (Turner 1968a)

$\Delta_c(t)$ = commercial correction factor (Turner 1968a)

Q_c = base commercial SO_2 emission rate

$F_c(t)$ = commercial diurnal variation factor

q_c = commercial heating SO_2 emission rate per degree

Q_v = river vessel SO_2 emission rate

Q_a = base automotive SO_2 emission rate

$F_a(t)$ = automotive diurnal variation factor

Q_w = railroad SO_2 emission rate

Q_b = backyard burning SO_2 emission rate

q_x = industrial heating SO_2 emission rate per degree

Q_p = base industrial process emission rate

$F_d(t)$ = industrial day of week variation factor

$F_h(t)$ = industrial diurnal variation factor

The parameters and variables in the above algorithm reflect a combination of basic data and assumptions. As a result, an attempt has been made to divide the above parameters into more fundamental components so that assumed and reported or observed values can be more easily identified. In the notation below subscripts i and j are introduced on parameters which vary from one area source to another. Subscript k denotes fuel types such as gas, oil and coal. Subscript a is used to designate an annual or national average.

$$(q_r)_{ij} = \frac{H_a\ R_{ij}}{D_a\ R_a} \sum_{k=1}^{K} \frac{S_k (N_k)_{ij}}{E_k\ H_k} \tag{10}$$

where H_a = average annual U.S. household space heating energy requirement

D_a = average annual U.S. degree days

R_a = average number of rooms per U.S. household

R_{ij} = average number of rooms per dwelling unit in grid square (i,j)

S_k = sulfur dioxide emitted per unit of fuel k

E_k = heating efficiency of fuel k

H_k = heat content of fuel k

$(N_k)_{ij}$ = number of residential dwelling units using fuel k in grid square (i,j)

K = number of fuels.

$$(Q_r)_{ij} = \frac{F_s}{1 - F_s} (q_r)_{ij}\ \overline{D_w} \tag{11}$$

where F_s = summer day fuel consumption as fraction of average winter day

$\overline{D_w}$ = average winter degree day.

$$(Q_c)_{ij} = \frac{1}{\Delta t_s} \sum_{k=1}^{K} S_k \sum_{\ell=1}^{C_{ij}} (F_s)_{k\ell}\ W_{k\ell} \tag{12}$$

where Δt_s = duration of season

C_{ij} = number of commercial sources in grid square (i,j)

$W_{k\ell}$ = annual quantity of fuel k used by ℓth source

$(F_s)_{k\ell}$ = fraction of annual quantity of fuel k used by ℓth source used in summer season

S_k = sulfur dioxide emitted per unit of fuel k.

$$(q_c)_{ij} = \frac{1}{D_w}\left\{\frac{1}{\Delta t_s}\left[\sum_{k=1}^{K} S_k \sum_{\ell=1}^{C_{ij}} (F_w)_{k\ell}\, W_{k\ell}\right] - (Q_c)_{ij}\right\} \tag{13}$$

where D_w = winter season degree days

$(F_w)_{k\ell}$ = fraction of annual quantity of fuel k used by ℓth source in winter season.

$$(q_x)_{ij} = \frac{1}{D_w} \sum_{k=1}^{K} S_k \sum_{\ell=1}^{I_{ij}} (F_w)_{k\ell}\, W_{k\ell} \tag{14}$$

where I_{ij} = number of industrial sources in grid square (i,j).

Thus the original algorithm may be written

$$\begin{aligned}
Q_{ij}(t) = {} & \left[\frac{F_s\, \overline{D_w}}{1 - F_s} + 65 - T(t)\right] - \Delta_r(t)\, \frac{H_a\, R_{ij}}{D_a\, R_a}\left[\sum_{k=1}^{K} \frac{S_k (N_k)_{ij}}{E_k\, H_k}\right] \\
& + \left[\frac{F_c(t)}{\Delta t_s} - \frac{65 - T(t) - \Delta_c(t)}{D_w}\right]\left[\sum_{k=1}^{K} S_k \sum_{\ell=1}^{C_{ij}} (F_s)_{k\ell}\, W_{k\ell}\right] \\
& + \frac{65 - T(t) - \Delta_c(t)}{D_w}\left[\sum_{k=1}^{K} S_k \sum_{\ell=1}^{C_{ij}} (F_w)_{k\ell}\, W_{k\ell}\right] \\
& + Q_v + Q_a\, F_a(t) + Q_w \\
& + Q_b + \frac{65 - T(t) - \Delta_c(t)}{D_w}\left[\sum_{k=1}^{K} S_k \sum_{\ell=1}^{I_{ij}} (F_w)_{k\ell}\, W_{k\ell}\right] \\
& + F_d(t)\, F_h(t) \sum_{\ell=1}^{I_{ij}} (Q_p)_\ell
\end{aligned} \tag{15}$$

In addition to the above emission information an estimate is provided of the effective height of each area source. Values were selected primarily on the basis of prevalent building heights in the area.

2.3 SUMMARY OF ST. LOUIS EMISSION PARAMETERS

Table B-2 lists the source parameters for estimating SO_2 emission rates for St. Louis point sources, the basis of the parameter estimate and the source of the information. Table B-3 shows the derived average diurnal variations in power plant SO_2 emission rates and plume rise factors for one plant with four emission sites. Table B-4 shows the diurnal variation in the commerical and residential temperature corrections for space heating requirements. Table B-5 lists the area source parameters available for estimating SO_2 emission rates for St. Louis area sources. As in Table B-2, the basis for the estimate and the source of information are also included. Table B-6 shows the diurnal variation in the commerical base emission factor and in the automotive emission factor. Miscellaneous additional emission parameters are listed in Tables B-7, B-8, and B-9.

Table B-2. Point Source Emission Data

Source Parameter	Basis of Estimate	Source of Information	Parameter Values
Q_p	Annual SO_2 emissions	Questionnaire	Stored on punched cards
$F_d(t)$	Usual days worked per week	Questionnaire	Stored (Saturday and Sunday listed as fraction of week day)
$F_h(t)$	Usual shifts worked per day	Questionnaire	Stored (midnight and swing shifts listed as fraction of day shift)
W_j	Annual fuel consumption	Questionnaire	Contained in q_x (stored on punched cards)
S_j	Chemical analyses		See Table B-8
D_a	Annual degree days	NOAA	Contained in q_x (stored on punched cards)
$(F_W)_j$	Percent W_j used in winter	Questionnaire	Contained in q_x (stored on punched cards)
Dw	Winter season degree days	NOAA	Contained in q_x (stored on punched cards)
Stack height	Stack height	Questionnaire	Stored on punched cards
Effective stack height	Stack height plus judgment	Questionnaire	Stored on punched cards
Plume rise-wind speed product	Stack diameter, exit gas temp. and flow rate		Stored on punched cards (also see Table B-3)
Q(t) for special power plant site	Fuel use, output loads	Plant oper.	See Table B-3
$\Delta_c(t)$	Temperature correlation with steam heat loads	Turner (1968a)	See Table B-4
T(t)	Airport hourly temp. obs.	NOAA	Stored on punched cards
L, L_ℓ, L_p	Plant output records	St. Louis Union Elec. Co.	Stored on punched cards (L_p, see Table B-1)
A_1, A_2	Plant operating characteristics	St. Louis Union Elec. Co.	See Table B-1
T_ℓ, T_u	Stack operating characteristics	St. Louis Union Elec. Co.	See Table B-1
V_ℓ, V_u	Stack operating characteristics	St. Louis Union Elec. Co.	See Table B-1

Table B-3. Diurnal SO_2 Emission Rates and Wind Speed - Plume Rise Products for Four Emission Sites of a St. Louis Power Plant

	Stack A		Stack B		Stack C		Stack D	
Two Period Ending	Emission Rate, g/sec	Wind Speed Plume Rise Product, m^2/sec	Emission Rate, g/sec	Wind Speed Plume Rise Product, m^2/sec	Emission Rate, g/sec	Wind Speed Plume Rise Product, m^2/sec	Emission Rate, g/sec	Wind Speed Plume Rise Product, m^2/sec
0200	106	40	106	40	282	102	1341	504
0400	106	40	106	40	282	102	1552	583
0600	106	40	106	40	282	102	2364	888
0800	106	40	106	40	600	217	2681	1007
1000	529	201	529	201	706	256	2681	1007
1200	423	161	529	201	706	256	2681	1007
1400	353	134	529	201	706	256	2681	1007
1600	212	80	529	201	706	256	2681	1007
1800	176	67	529	201	706	256	2681	1007
2000	318	120	529	201	706	256	2681	1007
2200	176	67	529	201	706	256	2681	1007
2400	106	40	106	40	282	102	1799	676

Table B-4. Diurnal Residential and Commercial Temperature Corrections (Turner, 1968a)

Hour Ending	$\Delta_c(t)$ Commercial Temperature Corrections, °F			$\Delta_r(t)$ Residential Temperature Corrections, °F		
	Weekday	Saturday	Sunday	Weekday	Saturday	Sunday
0100	13.32	17.03	16.87	11.11	10.08	8.11
0200	13.23	18.19	17.82	10.61	11.97	9.07
0300	12.54	16.30	18.43	9.69	9.69	9.12
0400	10.43	14.55	16.90	8.54	8.43	8.15
0500	5.64	10.17	15.15	7.08	6.65	6.64
0600	-1.75	3.19	12.86	3.13	4.24	4.76
0700	-8.04	-0.13	9.47	-2.15	1.85	1.83
0800	-11.69	-4.13	8.63	-7.32	-0.73	0.15
0900	-13.91	-7.14	6.01	-7.61	-6.30	-5.60
1000	-12.94	-6.74	4.82	-8.85	-8.01	-7.61
1100	-12.43	-7.00	2.64	-8.44	-7.26	-8.72
1200	-12.53	-6.98	1.38	-7.46	-9.34	-7.84
1300	-12.39	-7.11	0.30	-6.73	-8.28	-5.55
1400	-11.19	-7.01	0.55	-6.25	-8.07	-5.87
1500	-9.62	-3.84	2.98	-5.11	-7.78	-4.09
1600	-7.88	-1.84	4.49	-4.08	-6.14	-2.86
1700	-4.37	-0.66	6.25	-3.17	-5.28	-1.50
1800	0.56	2.60	8.70	-2.41	-3.82	-1.43
1900	4.55	5.97	9.92	-0.77	-1.73	-0.41
2000	6.62	7.92	10.10	-0.01	-0.86	-0.61
2100	9.08	8.90	10.47	2.56	2.31	-1.49
2200	10.41	11.47	12.01	3.22	3.85	-0.60
2300	11.53	13.48	12.23	5.33	5.71	1.23
2400	13.19	15.86	12.03	9.11	8.74	4.78

Table B-5. Area Source Emission Parameters

Source Parameter	Basis of Estimate	Source of Information	Parameter Values
F_s	Fuel company information	La Clede Gas Co.	0.2
H_a	National fuel data	Landsberg et al, 1963	70×10^6 Btu/yr
D_a	National meteorological data	Landsberg et al, 1963	4600 °F days/yr
N_a	Census information	Stat. Abstracts 1962	4.9 rooms/household
$(N_r)_{ij}$	1960 Census (St. Louis SMSA's)	U. S. Census Bureau	Contained in Q_r and q_r
$(N_{kr})_{ij}$	1960 Census (St. Louis SMSA's)	U. S. Census Bureau	Contained in Q_r and q_r
H_k	Assumed fuel heat content	Turner, 1968b	See Table B-7
E_k	Assumed combustion efficiency	Turner, 1968b	See Table B-7
S_k	Average fuel sulfur content	Turner, 1968b	See Table B-8
$F_c(t)$	Emission survey data	Not reported	See Table B-6
W_{kl}	Reported annual fuel use	Questionnaire	Contained in Q_c, q_c and q_x (stored on 1200 punched cards
$(Fs)_{kl}$	Reported % of W_{kl} used in summer	Questionnaire	Contained in Q_c and q_c (stored on 1200 punched cards)
$(Fw)_{kl}$	Reported % of W_{kl} used in winter	Questionnaire	Contained in q_c and q_x (stored on 1200 punched cards)
$(Qv)_{ij}$	Not reported	Not reported	Stored on 1200 punched cards
$(Qa)_{ij}$	Not reported	Not reported	Stored on 1200 punched cards
$F_a(t)$	Not reported	Not reported	See Table B-6
$(Qw)_{ij}$	Not reported	Not reported	Stored on 1200 punched cards
$(Qb)_{ij}$	Not reported	Not reported	Stored on 1200 punched cards
$[F_d(t)]_{ij}$	Usual industry working days	Questionnaire	Stored on 1200 punched cards
$[F_h(t)]_{ij}$	Usual industry working shifts	Questionnaire	Stored on 1200 punched cards
$(Q_p)_\ell$	Reported annual SO_2 emissions	Questionnaire	Contained in Q_p (stored on 1200 punched cards)
$\bar{D}_w$	1934 to 1964 St. Louis temp. data	NOAA	31.6°F
$T(t)$	Hourly airport temperature	NOAA	Stored on punched cards
$\Delta_r(t)$	Temperature correlations with gas sendouts	Turner, 1968a	See Table B-3

(Continued)

Table B-5. Area Source Emission Parameters (Concluded)

Source Parameter	Basis of Estimate	Source of Information	Parameter Values
$\Delta_c(t)$	Temperature correlations with steam heat loads	Turner, 1968a	See Table B-3
D_W	Winter season airport temperature	NOAA	Contained in q_c and q_x (stored on 1200 punched cards)
Source height	Estimate guided by building heights	Visual reports	Stored on 1200 punched cards

Table B-6. Base Commercial and Automotive Emission Factors for St. Louis Area Sources

Two Hour Period Ending	$F_c(t)$ Fraction of Mean Commercial Base Emission Rate	$F_a(t)$ Fraction of Mean Automotive Emission Rate
0200	0.20	0.176
0400	0.20	0.037
0600	0.20	0.111
0800	1.96	1.575
1000	1.82	2.261
1200	1.75	1.001
1400	1.69	0.788
1600	1.62	1.325
1800	1.48	2.632
2000	0.68	1.084
2200	0.20	0.573
2400	0.20	0.417

Table B-7. Miscellaneous Emission Parameters

Area Source Emission Data

1. Average energy use for space heating per household (USA wide) = 70×10^6 Btu/yr

   Ref: Resources in America's Future; H. H. Landberf, L.L. Fischran, J. T. Fisher; Johns Hopkins Press, 1963 (Baltimore, Md.).

2. Average degree days for the country = 4600 °F day/yr

   Ref: ditto (1)

3. Average size of household = 4.9 rooms/dwelling unit

   Ref: Statistical Abstracts of U.S.; 1962; Department of Commerce, Bureau of Census, Washington, D.C.

4. Fossil fuel characteristics:

Fuel	Heat Content (H_k)	Combustion Efficiency (E_k)
Coal	26×10^6 Btu/ton	0.5
Oil	145,000 Btu/gal	0.6
Gas	1,000 Btu/ft^3	0.75

5. Summer fuel use = 20% of winter day

6. Average St. Louis winter degree day = 31.6 °F day

   Ref: Dec, Jan, Feb 1934 to 1964 Weather Bureau records.

7. Information from U.S. Census of Housing (estimated from SMSA data) obtained for source area:

   (a) Number of dwelling units
   (b) Rooms per dwelling unit
   (c) Number of coal burning units
   (d) Number of gas burning units
   (e) Number of oil burning units
   (f) Population.

8. Survey questionnaire information requested in St. Louis Intrastate State Study (Turner 1968b):

   (a) Source Location
   (b) Type of fuel and annual use required
   (c) Percent used by season
   (d) Stack height
   (e) Process emissions in tons per year.

Table B-8. St. Louis SO_2 Emission Parameters

Fuel	Fuel Requirements		SO_2 Emission			
	For average U. S. household (4-9 rooms/ household), units per household per degree day	For average U. S. room, units per room per degree day	SO_2 emission lb SO_2 per unit (S_k)	SO_2 heating emission rate, grams per second per room per degree (a)	St. Louis Values	
					Sulfur content	SO_2 heating emission rate, grams per second per room per degree (a)
Coal	0.0012 tons	2.45×10^{-4} tons	38p per ton	$4.88p \times 10^{-5}$	3.3%	1.61×10^{-4}
Oil	0.18 gal	3.67×10^{-2} gal	157p per 10^3 gal	$3.025p \times 10^{-5}$	1.5%	4.54×10^{-5}
Gas	22.5 ft^3	4.59 ft^3	2.86s per 10^2 ft^3	$6.89s \times 10^{-8}$	0.3 grains per 10^2 ft^3	2.08×10^{-8}

p = % sulfur content by weight
s = grains sulfur content per 100 ft^3

(a) degree = number degrees average outside temperature is below 65°F

Table B-9. Average Sulfur Content of Coal Used by St. Louis Power Plants

Plant	Sulfur Content, %
Meramec	2.86
Venice	2.52
Cahokia	1.96
Ashley	3.39

Section 3.0

METEOROLOGICAL DATA

The following meteorological data were obtained for the St. Louis area:

1. Hourly Lambert Field aviation weather observations
2. Hourly Scott Field aviation weather observations
3. Lindbergh High School wind, temperature and relative humidity hourly averages from strip charts
4. State Police Station C hourly averages of wind, temperature and relative humidity
5. Hazelwood High School hourly averages of wind, temperature and relative humidity
6. TV tower hourly averages of temperature and wind at 3 heights and a bivane measured standard deviation in wind direction.

The parameters and units which are available on punch cards are listed in Tables B-10 and B-11.

Table B-10. Summary of St. Louis Hourly Airport Weather Observations (Available for Lambert Field and Scott Field)

Parameter	Units
Ceiling	Hundreds of Feet or Code
Sky Cover	Code
Visibility	Tenths of Mile
Weather Elements	Code
Temperature	°F
Dew Point	°F
Wind Direction	Tens of Degrees
Wind Speed	Knots
Peak Gust	Knots
Altimeter Setting	Hundredths of Inches of Mercury
Precipitation (Lambert Field Only)	Hundredths of Inches

Table 11. Hourly Average Weather Observations

Observation Point	Parameter	Units
Lindbergh HS	Wind speed	Miles per hour
Lindbergh HS	Wind direction	Tens of degrees
Lindbergh HS	Temperature	°F
Lindbergh HS	Relative humidity	%
State Patrol Station C	Wind speed	Miles per hour
State Patrol Station C	Wind direction	Tens of degrees
State Patrol Station C	Temperature	°F
State Patrol Station C	Relative humidity	%
Hazelwood HS	Wind speed	Miles per hour
Hazelwood HS	Wind direction	Tens of degrees
Hazelwood HS	Temperature	°F
Hazelwood HS	Relative humidity	%
TV Tower, 127 ft	Wind speed	Miles per hour
TV Tower, 127 ft	Wind direction	Tens of degrees
TV Tower, 255 ft	Wind speed	Miles per hour
TV Tower, 255 ft	Wind direction	Tens of degrees
TV Tower, 459 ft	Wind speed	Miles per hour
TV Tower, 459 ft	Wind direction	Tens of degrees
TV Tower 124 ft	Temperature	°F
TV Tower	124 ft to 249 ft temperature gradient	°F
TV Tower	124 ft to 452 ft temperature gradient	°F
TV Tower	249 ft to 452 ft temperature gradient	°F
TV Tower	Bivane standard deviation	degrees

Section 4.0

AIR QUALITY DATA

Two types of SO_2 measurements are available for St. Louis. Ten stations with average two-hour observations are available, and 40 stations with average 24-hour observations are available. The sampling period for 24-hour observations began and ended at 2 p.m. daily. This time of day permits bubbler collectors to be switched at a time when ambient concentrations are expected to be a minimum. Both 2-hour and 24-hour samplers used a bubbler collection assembly to measure SO_2 concentrations. The basic National Air Sampling Network (NASN) gas sampling bubbler, with slight modifications, was used. Each bubbler consisted of a polypropylene centrifuge tube (4 inches long by 1 inch diameter) fitted with a two-hole rubber stopper. A glass tube extended to approximately 5/16-inch from the bottom of the bubbler tube. The airflow was regulated with a standard Gelman orifice assembly. Flow rate determinations were made weekly with a calibrated flow meter. In the two-hour samplers approximately 120 liters of air was bubbled through the sampler each two hours. An external vacuum pump draws air through the bubbler where sulfur dioxide is stripped from the air stream by the complexing action of sodium tetrachloro-mercurate absorbing reagent. The collected samples were transported to a laboratory where they were analyzed for SO_2 concentrations. Twelve two-hour samples were picked up for analysis each day and analyzed in a specially set up local laboratory. The analytical method used was that of West and Gaeke as modified by Welch and Terry. Duplicate sets of 24-hour samples were available at the same locations as the two-hour samples. A comparison of the 24-hour concentrations measured by two-hour samplers and by the 24-hour samplers revealed that two-hour samplers averaged about 15 percent higher than the 24-hour samplers.

Section 5.0

ST. LOUIS PREPROCESSING PROGRAM LISTINGS

```
C ST LOUIS DATA
      DIMENSION TFR(24,3),TFCI(24,3),DFC(24),DFA(24),SULFR(7),PLOAD(8)
      DIMENSION HA(1200),Z(3),TFR2(24),TFCI2(24),HA2(380)
      DIMENSION XR(50),YR(50),ZR(50),OBSO2(50) ,XP(51),YP(51)
      DIMENSION ZP(51),QP(51),CASO2(40),QB(1200),QRH(1200),QCB(1200),
     1QCIH(1200),QAU(1200),QSA(1200),SATA(1200),SUNA(1200),SMIDA(1200),
     2 SWIGA(1200),QIJ(3600)
      EQUIVALENCE (TFR2(1),TFR(1,3)),(TFCI2(1),TFCI(1,3)),(HA2(1),HA(821
     1))
      DATA DLAST/22814./
      DATA NH/3/
      DATA Z/20.,30.,45./
      DATA DLTA/1524./
      DATA NRECP/50/
      DATA NR1/40/
      DATA CASO2/40*0./
      DATA GX/30./
      DATA GY/40./
      DATA NIPS/44/
      DATA NUS/7/
      DATA NRPNT/51/
      DATA XP / 3.94, 9.32,14.04,14.88,14.60,19.20,18.76,20.26,19.92,
     1         20.84,22.00,24.88,24.58,26.52,31.00,16.52,16.96,13.84,
     2         16.08,15.46,18.00,18.14,18.38,19.14,20.88,20.86,21.14,
     3         20.96,21.90,21.82,21.88,21.62,22.72,24.46,23.54,24.62,
     4         26.14,29.86,18.16,18.68,22.34,22.36,22.38,22.40,10.84,
     5         10.80,10.76,10.74,19.88,19.41,19.67/
      DATA YP /13.20,28.80,26.88,12.34,13.50,18.20,22.66,17.06,16.52,
     1         38.14,19.56,34.76,34.70,34.66,30.20,21.56,15.84, 8.66,
     2         18.90,23.00,17.00,17.00,21.58,21.84,16.88,24.30,25.00,
     3         24.80,17.64,24.14,37.66,37.98,19.40,20.82,38.30,35.84,
     4         34.72,11.08,18.34,19.08,36.52,36.52,36.52,36.52, 2.84,
     5          2.85, 2.86, 2.87,21.78,17.50,19.87/
      DATA HA/343*20.,30.,29*20.,2*30.,29*20.,30.,22*20.,3*30.,3*20.,3*
     1 30.,20*20.,4*30.,2*20.,5*30.,21*20.,10*30.,21*20.,10*30.,20.,3*
     2 30.,16*20.,8*30.,2*40.,20.,4*30.,16*20.,2*30.,2*20.,3*30.,40.,50.
     3,3*20.,3*30.,15*20.,7*30.,2*40.,20.,30.,20.,3*30.,15*20.,9*50.,21*
     4 20.,8*30.,2*20.,30.,19*20.,30.,2*20.,3*30.,23*20.,2*30.,3*20.,2*
     5 30.,4*20.,3*30.,16*20.,30.,4*20.,30.,20.,30.,23*20.,3*30.,27*20./
      DATA HA2    /3*30.,29*20.,30.,221*20.,30.,28*20.,2*30.,26*30.,30.,
     1 20.,30.,27*20.,30.,38*20./
      DATA XR/19.42,20.16,18.66,20.24,17.72,21.18,18.12,20.76,16.22,20.4
     18,16.52,22.48,18.04,22.32,16.32,20.42,14.14,21.02,14.16,22.44,14.9
     26,24.14,16.88,20.24,18.50,18.88,15.42,22.30,13.78,23.26,11.14,24.7
     36,10.34,27.10,10.68,26.04,13.96,23.54,14.74,16.64,18.66,16.32,14.1
     44,16.88,10.34,20.24,20.48,22.48,22.30,26.04/
      DATA YR/     20.86,20.06,19.16,22.36,20.14,21.20,22.50,19.20,21.16,
     117.88,18.92,18.64,17.76,16.64,24.12,25.20,21.46,23.84,20.26,20.64,
     218.04,19.78,15.88,15.80,28.42,14.94,27.88,26.86,25.06,25.04,23.64,
     323.22,20.34,19.98,17.18,17.06,16.06,14.52,14.32,13.04,19.16,24.12,
     421.46,15.88,20.34,22.36,17.88,18.64,26.86,17.06/
      DATA ZR/50*0./
      DATA TFR/  8.11,  9.07,  9.12,  8.15,  6.64,  4.76,  1.83,  0.15,
     1          -5.60, -7.61, -8.72, -7.84, -5.55, -5.87, -4.09, -2.86,
     2           1.50, -1.43, -0.41, -0.61, -1.49, -0.60,  1.23,  4.78,
     3          11.11, 10.61,  9.69,  8.54,  7.08,  3.13, -2.15, -7.32,
     4          -7.61, -8.85, -8.44, -7.46, -6.73, -6.25, -5.11, -4.08,
     5          -3.17, -2.41, -0.77, -0.01,  2.56,  3.22,  5.33,  9.11/
      DATA TFR2/
     6          10.08, 11.97,  9.69,  8.43,  6.65,  4.24,  1.85, -0.73,
     7          -6.30, -8.01, -7.26, -9.34, -8.28, -8.07, -7.78, -6.14,
     8          -5.28, -3.82, -1.73, -0.86,  2.31,  3.85,  5.71,  8.74/
      DATA TFCI/16.87, 17.82, 18.43, 16.90, 15.15, 12.86,  9.47,  8.63,
     1           6.01,  4.82,  2.64,  1.38,  0.30,  0.55,  2.98,  4.49,
     2           6.25,  8.70,  9.92, 10.10, 10.47, 12.01, 12.23, 12.03,
     3          13.32, 13.23, 12.54, 10.43,  5.64, -1.75, -8.04,-11.69,
     4         -13.91,-12.94,-12.43,-12.53,-12.39,-11.19, -9.62, -7.88,
     5          -4.37,  0.56,  4.55,  6.62,  9.08, 10.41, 11.53, 13.19/
```

```
      DATA TFCI2/
     6          17.03, 18.19, 16.30, 14.55, 10.17,  3.19, -0.13, -4.13,
     7          -7.14, -6.74, -7.00, -6.78, -7.11, -7.01, -3.84, -1.84,
     8          -0.66,  2.60,  5.97,  7.92,  8.90, 11.47, 13.48, 15.86/
      DATA DFC/0.200,0.200,0.200,0.200,0.200,0.200,1.960,1.960,
     1         1.820,1.820,1.750,1.750,1.690,1.690,1.620,1.620,
     2         1.480,1.480,0.680,0.680,0.200,0.200,0.200,0.200/
      DATA DFA/0.176,0.176,0.037,0.037,0.111,0.111,1.575,1.575,
     1         2.261,2.261,1.001,1.001,0.788,0.788,1.325,1.325,
     2         2.632,2.632,1.084,1.084,0.573,0.573,0.417,0.417/
      DATA SULFR/4*2.863,2.517,1.963,3.394/
      DATA IR1/5/
      DATA IW1/6/
C XR,YR VALUES IN LOCATIONS 41-50 ARE THE LOCATIONS FOR THE 2HR SAMPLERS
C  IN THE SEQUENCE THE 2HR CONC OBS ARE LISTED ON THE DATA CARDS
C SULFR DATA IS THE MEAN VALUE OF 12 WEEK PERIOD
C  INPUT OUTPUT DEVICE NUMBERS USED AS FOLLOWS
C               IR1 CARD READER
C               IW1 ON LINE PRINTER
      REWIND 10
      REWIND 11
      REWIND 12
      REWIND 13
      REWIND 14
      REWIND 15
      REWIND 16
      IR1 = 5
      READ(IR1,9000)   IH1,IH2
 9000 FORMAT(10I5)
      DO 1 I=1,NRPNT
      XP(I) = 1524. * XP(I)
      YP(I) = 1524. * YP(I)
    1 CONTINUE
      CALL INA(QB,QRH,QCB,QCIH,QAU,QSA,SATA,SUNA,SMIDA,SWIGA,IR6,GX,GY)
      II = IH1 - 1
       IF (II) 8,8,2
    2 CONTINUE
      DO 3 I=1,II
      READ (10)
      READ (11)
      READ (15)
      READ (16)
    3 CONTINUE
      II = II/24
      IF (II)  8, 8,12
   12 CONTINUE
      DO 13 I=1,II
      READ (12)
   13 CONTINUE
      II = (IH1 - 1)/2
      IF (II) 8,8,14
   14 CONTINUE
      DO 15 I=1,II
      READ (13)
   15 CONTINUE
    8 CONTINUE
      DO 2000 IRR = IH1,IH2
      JN = IRR
C  READ MET DATA
      CALL METIN( JN,YMDH,YEAR,AMNTH,DAY,HOUR,IDOW,WS,WH,P,WD,
     1 INDEX,CIGMX,SIGA,RIB,PCPN,WGLD,STAPR,TG, TEMP)
      IF (I - 614) 11,10,11
   10 CONTINUE
      YMDH = 2704.
   11 CONTINUE
C  LOAD EMISSION DATA
      CALL SHIFT(ID,IS,IDOW,HOUR)
      IH = HOUR
      DDR = 65. - (TEMP + TFR(IH,ID))
      IF (DDR) 4,5,5
    4 DDR = 0.
    5 CONTINUE
      DDC = 65. - (TEMP + TFCI(IH,ID))
      IF (DDC) 6,7,7
    6 DDC = 0.
    7 CONTINUE
      CALL IEMIT(NIPS,WS,WH,P,DDC,IS,ID,IH,CIGMX,TG,ZP,QP)
C  CALL INPUT ROUTINE TO READ PLOAD DATA -INPLD
      CALL INPLD( JN,PLOAD,PMDH)
      IF( PMDH - YMDH) 100,200,100
  100 CONTINUE
      WRITE(IW1,9200)YMDH,YEAR,PMDH
 9200 FORMAT('0 DATE TIME GROUP FROM PLOAD DATA AND MET DATA DO NOT MATC
     1H*** MET DATA YMDH= ',F7.0,'  YEAR= ',F3.0,/,58X,' PLOAD DATE GROU
     2P= ',F7.0,///)
  200 CONTINUE
      PLOAD(7) = PLOAD(7) * 14.07 + 20. + PLOAD(8)
      IU = NIPS + 1
      CALL UEMIT(NIPS,NUS,TEMP,STAPR,TG,WS,WH,P,PLOAD,SULFR,CIGMX,ZP(IU)
     1,QP(IU))
      CALL AEMIT(HA,GX,GY,ID,IS,DDR,DDC,DFC(IH),DFA(IH),QB,QRH,QCB,QCIH,
     1QAU,QSA,SATA,SUNA,SMIDA,SWIGA,QIJ)
C  DETERMINE IF HOUR OF DATA IS ODD OR EVEN--IF ODD FILL THE SO2 ARRAY
C  WITH ZEROS IF EVEN READ THE 2 HR SO2 OBS
      DO 1300  NEO = 2,24,2
      FNEO = NEO
      IF (HOUR -FNEO) 1300,1400,1300
 1300 CONTINUE
      DO 1310 I=1,NRECP
      OBSO2(I) = 0
 1310 CONTINUE
      GO TO 1200
 1400 CONTINUE
C  SUBROUTINE NSO2 READS IN THE 2HRLY SO2 OBSERVATIONS
      CALL NSO2( JN,OBSO2,SMDH3,NR1,NRECP)
      IF (SMDH3 - 120000.) 1420,1410,1410
 1410 CONTINUE
      SMDH3 = SMDH3 - 120000.
 1420 CONTINUE
C  CHECK 2HRLY DTG WITH MET DATA YMDH FOR CORRECT SO2 OBS.
      IF ( YMDH - SMDH3) 1500,1700,1500
 1500 CONTINUE
C  WRITE ERROR MESSAGE FOR NONMATCHING DTG FROM 2 HR SO2 OBS
      WRITE (IW1,9600) SMDH3,YMDH
 9600 FORMAT ('0 DATE-TIME FROM 2HR SO2 OBS DOES NOT MATCH DATE-TIME OF
     1 MET DATA -  DTG FROM SO2 IS ',F7.0,' DTG OF MET. IS ',F7.0///)
 1700 CONTINUE
      IF(HOUR - 14.) 1100,300,1100
  300 CONTINUE
C CALL IN 24 HOUR SO2 OBSERVATIONS WITH DTG READ FROM EACH CARD
      CALL NSO24 ( JN,OBSO2,SMDH1,NR1)
      DTGC = SMDH1 - 120000.
      IF (DTGC ) 1000,1000,800
  800 CONTINUE
      IF ( DTGC - YMDH) 900,1200,900
  900 CONTINUE
      WRITE (IW1,9500) SMDH1,YMDH
 9500 FORMAT ('0 DATE-TIME OF 24 HR SO2 DATA READ BY NSO24 DOES NOT MATC
     1H DATE-TIME OF MET. DATA  SO2 DTG= ',F7.0,'   MET DTG= ',F7.0,///)
      GO TO  1200
 1000 CONTINUE
      IF ( YMDH - SMDH1) 900,1200,900
 1100 CONTINUE
      DO 1110 I=1,NR1
      OBSO2(I) = 0
 1110 CONTINUE
 1200 CONTINUE
        CALL      HROUT (IW2,YMDH,YEAR,AMNTH,DAY,IDOW,HOUR,WS,WH,P,WD,
     1 INDEX,CIGMX,SIGA,RIB,PCPN,WGLD,STAPR,TG, TEMP,NRECP,NR1,XR,YR,
     2 ZR,OBSO2,CASO2,GX,GY,DLTA,NH,Z,NRPNT,XP,YP,ZP,QP)
       CALL OUTA(YMDH,GX,GY,NH,QIJ,IW3)
       WRITE (IW1,9700) YMDH
 9700 FORMAT (' RECORD WITH INDEX =', F10.0,', WRITTEN ON UNIT 15 AND 16
     1')
       IF (YMDH - DLAST) 1800,2100,2100
 1800 CONTINUE
 2000 CONTINUE
 2100 CONTINUE
       END FILE 15
       END FILE 16
       REWIND 10
       REWIND 11
       REWIND 12
       REWIND 13
       REWIND 14
       REWIND 15
       REWIND 16
       CALL EXIT
       END


       SUBROUTINE AEMIT(HA,GX,GY,ID,IS,DDR,DDC,DFC,DFA,QB,QRH,QCB,QCIH,
     1QAU,QSA,SATA,SUNA,SMIDA,SWIGA,QIJ)
C THIS ROUTINE COMPUTES A THREE DIMENSIONAL ARRAY OF EMISSION RATES FOR
C AREA SOURCE
       DIMENSION QIJ(1),HA(1),QB(1),QRH(1),QCB(1),QCIH(1),QAU(1),QSA(1),
     1SATA(1),SUNA(1),SMIDA(1),SWIGA(1)
       NI = GX * GY
       DO 20 I=1,NI
C GET DAY-OF-WEEK EMISSION FACTOR
       GO TO (1,2,3),ID
    1 DOWF = SUNA(I)
       GO TO 4
    2 DOWF = 1.
       GO TO 4
    3 DOWF = SATA(I)
    4 CONTINUE
C GET HOUR-OF-DAY EMISSION FACTOR
       GO TO (5,6,7),IS
    5 SHFTF = SMIDA(I)
       GO TO 8
    6 SHFTF = 1.
       GO TO 8
    7 SHFTF = SWIGA(I)
    8 CONTINUE
       QA = QB(I) + QRH(I) * DDR + QCB(I) * DFC + QCIH(I) * DDC + QAU(I)
     1 * DFA + QSA(I) * DOWF * SHFTF
       QIJ(I) = 0.
       K = I + NI
       QIJ(K) = 0.
       L = K + NI
       QIJ(L) = 0.
       IF (HA(I) - 30.) 9,10,11
    9 QIJ(I) = QA
       GO TO 12
   10 QIJ(K) = QA
       GO TO 12
   11 QIJ(L) = QA
   12 CONTINUE
   20 CONTINUE
       RETURN
       END
```

```
      SUBROUTINE UEMIT(NIPS,NUS,TBAR,PRESS,TG,U1,Z1,P,PLOAD,SULFR,CIGMX,
     1ZP,QP)
C                                    THIS ROUTINE COMPUTES EMISSION RATE (
C AND EFFECTIVE HEIGHT (ZP) FOR UTILITY POINT SOURCES
C USES INPUTS
C               TBAR   -  AIR TEMPERATURE, DEG K
C              PRESS   -  AIR PRESSURE, IN HG
C               NUS    -  NUMBER OF STACKS
C              PLOAD   -  POWER LOAD, MEGAWATTS
C              SULFR   -  SULFUR CONTENT OF FUEL, PERCENT
C                  A   -  PARAMETERS OF FUEL - LOAD RELATIONSHIP,LB/MIN -
C                  B   -  PARAMETERS OF FLUE GAS TEMP - LOAD RELATIONSHIP,
C                  C   -  PARAMETERS OF FLUE GAS FLOW RATE - LOAD RELATION
      DIMENSION A(3,7),B(4,7),C(4,7),PLOAD(1),SULFR(1),HPT(7),ZP(1),
     1QP(1)
      DATA EMIS/2./,FCON/0.075598/
      DATA A/ 50.,10.89 , 150., 50.,10.89 , 150.,100.,10.43 , 300.,
     1        100.,10.75 , 405., 20.,13.   , 480.,  0.,16.67 , 150.,
     2          0., 1.536,1500./
      DATA B/281.,294.,312.,343.,281.,294.,312.,343.,242.,262.,290.,336.
     1,       236.,267.,323.,372.,252.,293.,312.,352.,350.,406.,420.,434.
     2,       296.,323.,342.,356./
      DATA C/ 40.,170.,320.,500., 40.,170.,320.,500.,210.,375.,625.,
     11015.,260.,490.,840.,1460.,30.,625.,1180.,1840.,20.,260.,520.,835.
     2,         5.,225.,440., 665./
      DATA HPT/2*76.5,2*106.7,72.3,100.3,56.2/
C CONVERT TBAR FROM DEG F TO DEG K
      TEMP = (TBAR - 32) / 1.8 + 273.
C EMIS = GM SO2 EMITTED PER GM SULFUR IN FUEL ANALYSIS
C FCON = FUEL UNIT CONVERSION FACTOR = (GM/LB) * (MIN/SEC) * (1./100PER
      QCON = EMIS * FCON
      DO 20 I=1,NUS
C COMPUTE SO2 EMISSION
      IF (PLOAD(I)) 2,2,3
    2 QP(I) = 0.
      GO TO 4
    3 CONTINUE
      FUEL = A(1,I) + A(2,I) * PLOAD(I)
      QP(I) = QCON * SULFR(I) * FUEL
    4 CONTINUE
C COMPUTE FLUE GAS TEMPERATURE (DEG K) AND FLOW RATE (CU.CM/SEC)
      CHKLD = PLOAD(I) / A(3,I)
      PLFR = CHKLD - 0.66667
      IF (PLFR) 10,13,13
   10 PLFR = CHKLD - 0.33333
      IF (PLFR) 11,12,12
   11 K2 = 2
      FR = 3. * CHKLD
      GO TO 15
   12 K2 = 3
      GO TO 14
   13 K2 = 4
   14 FR = 3. * PLFR
   15 K1 = K2 - 1
      STKTP = (B(K1,I) + FR * (B(K2,I) - B(K1,I)) - 32.) / 1.8 + 273.
      STKFL = (C(K1,I) + FR * (C(K2,I) - C(K1,I))) * 471.95E3
C COMPUTE HEAT EMISSION
C CONSTANT .00206495=2.553(SP.HEAT(CONST.VOL)/GAS CONST)*33863.9(DYNE/SQ
C                     IN.HG(32F))*2.38848E-8(CAL/DYNE CM)
      QHEAT = 0.00206495 * PRESS * STKFL * (STKTP - TEMP) / STKTP
      WS = U1 * (HPT(I) / Z1)**P
      CALL PLUMZ(TG,QHEAT,TEMP,HPT(I),WS,ZP(I),QP(I),CIGMX)
   20 CONTINUE
      RETURN
      END
      SUBROUTINE IEMIT(NIPS,U1,Z1,P,DDC,IS,ID,IH,CIGMX,TG,ZP,QP)
C                                THIS ROUTINE COMPUTES EMISSION RATE
C AND EFFECTIVE HEIGHT (ZP) FOR INDVSTRIAL POINT SOURCES
      DIMENSION ZP(1),QP(1)
      DIMENSION QSI(44),QSI2(4),QHI(44),HPT(44),UDH(44)
      DIMENSION SAT (44),SUN (44),SWIG (44),SMID (44)
      DIMENSION Q(12,4),UDHS(12,4)
      EQUIVALENCE (QSI(37),QSI2(1))
      DATA QHI/190.86,575.63, 75.45, 74.60,  1.29,200.31, 17.82,203.19,
     1          60.00,  0.00,361.00,  0.00, 22.70,  7.24,  7.66, 15.25,
     2          31.19, 09.01,101.23,189.38, 69.44,  0.00,  0.11,141.83,
     3          20.73,238.94,  0.00, 22.32, 27.86,279.60,798.18,176.01,
     4           6.78,  3.62,390.81,533.55,  0.00,  0.00, 24.95, 62.37/
      DATA QSI/   .0383, 35.0118,   .0009,397.5426, 16.7393, 94.1626,
     1          24.8305,390.6217,18.9670, 19.3968,  0.0   , 33.3890,
     2           7.5876, 73.3152,  3.2161, 10.7800,  4.1580, 10.3950,
     3          57.6870, 20.2691,  0.0   ,305.3670, 60.9396, 63.6274,
     4           7.8490, 31.5156,162.7519,  4.9417, 26.3866,911.3780,
     5           0.2635, 35.2936, 73.1896, 20.2018, 18.7807,334.0416/
      DATA QSI2/585.5721,25.6327, 23.1000, 12.9362/
      DATA HPT /40.,20.,7*40.,15.,20.,4*40.,49.,19.,47.,4*75.,2*55.,
     1          3*75.,2*55.,2*75.,2*55.,75.,3*55.,75.,59.,64.,3*76.2,
     2          107.5/
      DATA UDH /0.,806.,0.,287.,0.,246.,0.,428.,2*0.,487.,10*0.,218.,0.,
     1          77.,0.,97.,106.,2*0.,202.,402.,3*0.,101.,650.,1030.,3*0./
      DATA SAT/3*0.,1.,.99, 1.,0.,1.,0.,1.,0.,1.,0.,1.,0.,3*1.,3*0.,2*1.
     1        ,0.,1.,0.,1.,0.,6*1.,0.,2*1.,0.,2*1./
      DATA SUN/3*0.,1.,.99, 1.,0.,1.,0.,1.,0.,1.,0.,1.,0.,3*1.,3*0.,2*1.
     1        ,0.,1.,0.,1.,0.,6*1.,0.,2*1.,0.,2*1./
      DATA SWIG /4*1.,.99,13*1.,0.,8*1.,.48,12*1./
      DATA SMID /2*0.,2*1.,.99,5*1.,0.,1.,0.,5*1.,3*0.,6*1.,.48,9*1.,0.,
     1          2*1./
      DATA Q/4*106.,529.,423.,353.,212.,176.,318.,176.,5*106.,7*529.,
     1 106.,3*282.,600.,7*706.,282.,1341.,1552.,2364.,8*2681.,1799./
      DATA UDHS/4*40.,201.,161.,134.,80.,67.,120.,67.,5*40.,7*201.,40.,
     1 3*102.,217.,7*256.,102.,504.,583.,888.,8*1007.,676./
      DATA ISTAR/0/
      IF (ISTAR) 31,29,31
   29 CONTINUE
      ISTAR = 1
      DO 30 I=1,40
      QHI(I) = 0.01 * QHI(I)
   30 CONTINUE
   31 CONTINUE
      DO 10 I=1,NIPS
      J = I - 40
      IF (J) 20,20,15
   15 CONTINUE
      QHI(I) = 0
      SAT(I) = 1.
      SUN(I) = 1.
      SWIG(I) = 1.
      SMID(I) = 1.
      I1 = (IH + 1) / 2
      QSI(I) = Q(I1,J)
      UDH(I) = UDHS(I1,J)
   20 CONTINUE
C GET DAY-OF-WEEK EMISSION FACTOR, 1=SUNDAY, 2=WEEKDAY, 3=SATURDAY
      GO TO (1,2,3),ID
    1 DOWF = SUN(I)
      GO TO 4
    2 DOWF = 1.
      GO TO 4
    3 DOWF = SAT(I)
    4 CONTINUE
```

```
C GET HOUR-OF-DAY EMISSION FACTOR, 1=01-08, 2=09-16, 3=17-24
      GO TO (5,6,7),IS
    5 SHFIF = SMID(I)
      GO TO 8
    6 SHFTF = 1.
      GO TO 8
    7 SHFTF = SWIG(I)
    8 CONTINUE
      QP(I) = QHI(I) * DDC + QSI(I) * DOWF * SHFTF
      WS = U1 * (HPT(I) /Z1)**P
      ZP(I) = UDH(I)/ WS + HPT(I)
      IF (TG - 999.) 9,13,9
    9 IF (TG) 13,13,11
   11 CONTINUE
      ANUM = UDH(I) / (2.9 * WS)
      DZCRI = 2. * ANUM * SQRT(ANUM * (TG + 0.0098) / (TG * CIGMX))
      IF (CIGMX - HPT(I) - DZCRI) 12,12,13
   12 QP(I) = 0
   13 CONTINUE
   10 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SHIFT(ID,IS,KDOW,HOUR)
C DETERMINE DAY OF WEEK
      IF (KDOW - 2)  5,6,7
C SUNDAY AND HOLIDAY
    5 ID = 1
      GO TO 9
C WEEKDAY
    6 ID = 2
      GO TO 9
    7 IF (KDOW - 7) 6,8,5
C SATURDAY
    8 ID = 3
    9 CONTINUE
C DETERMINE SHIFT
      IF (HOUR - 9.) 10,11,11
C MIDNIGHT SHIFT (01 - 08)
   10 IS = 1
      GO TO 14
   11 IF (HOUR - 17.) 12,13,13
C DAY SHIFT (09 - 16)
   12 IS = 2
      GO TO 14
C SWING SHIFT (17 - 24)
   13 IS = 3
   14 CONTINUE
      RETURN
      END
      SUBROUTINE HROUT (IW2,YMDH,YEAR,AMNTH,DAY,IDOW,HOUR,WS,WH,P,WD,
     1 INDEX,CIGMX,SIGA,RIB,PCPN,WGLD,STAPR,TG,AVTMP,NRECP,NR1,XR,YR,
     2 ZR,OBSO2,CASO2,GX,GY,DLTA,NH,Z,NRPNT,XP,YP,ZP,QP)
      DIMENSION   XR(1),YR(1),ZR(1),OBSO2(1),Z(1),XP(1),YP(1),ZP(1),QP(1)
     1,CASO2(1)
      WRITE(15)     YMDH,YEAR,AMNTH,DAY,IDOW,HOUR,NRECP,NR1,(XR(N),N=1,
     1 NRECP),(YR(N),N=1,NRECP),(ZR(N),N=1,NRECP),(OBSO2(N),N=1,NRECP),
     2 (CASO2(N),N=1,NR1),
     3  GX,GY,DLTA,NH,(Z(N),N=1,NH),NRPNT,(XP(N),N=1,NRPNT),(YP(N),N=1,
     4 NRPNT),(ZP(N),N=1,NRPNT),(QP(N),N=1,NRPNT),WS,WH,P,WD,INDEX,
     5 AVTMP,CIGMX,SIGA,RIB,PCPN,WGLD,STAPR
      RETURN
      END
```

```
      SUBROUTINE INA (QB,RH,CB,QCIH ,AUM,QBA,SATA,SUNA,SMIDA, SWGA,IO1,
     1GX,GY)
      DIMENSION QB(1),RH(1),CB(1),QCIH(1),     AUM(1),QBA(1),
     1             SATA(1),SUNA(1),SWGA(1),SMIDA(1)
      NG = GX * GY
      DO 100 I= 1,NG
      READ(14)    RB,RH(I),CB(I),CH,VM,AUM(I),RRM,BBM,
     1 QBA(I),QHA    ,SATA(I),SUNA(I),SWGA(I),SMIDA(I)
      QB(I) = RB + VM + RRM + BBM
      QCIH(I) = CH + QHA
  100 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE INPLD (IR2,PLOAD,PMDH)
      DIMENSION PLOAD(1)
      READ(11)       PMDH,(PLOAD(N),N=1,8)
      RETURN
      END
```

```
      SUBROUTINE METIN(IR5,YMDH,YEAR,AMNTH,DAY,HOUR,IDOW,WS,WH,P,WD,
     1 INDEX,CIGMX,SIGA,RIB,PCPN,WGLD,STAPR,TG,AVTMP )
      READ( 10)      YMDH,YEAR,AMNTH,DAY,HOUR,IDOW,WS,WH,P,WD,
     1 INDEX,CIGMX,SIGA,RIB,PCPN,WGLD,STAPR,TG,AVTMP
      RETURN
      END
```

```
      SUBROUTINE NSO2( IR4,OBSO2,SMDH3,NR1,NRECP)
      DIMENSION OBSO2(1)
      N1 = NR1 + 1
      READ (13)          SMDH3,( OBSO2(N),N=N1,NRECP)
      RETURN
      END
      SUBROUTINE NSO24(IR3,OBSO2, SMDH1,NR1)
      DIMENSION OBSO2( 1)
      READ (12)    SMDH1,(OBSO2(N),N=1,NR1)
      RETURN
      END


      SUBROUTINE OUTA(YMDH,GX,GY,NH,QIJ,IW3)
      DIMENSION QIJ(1)
[illegible] = GX * GY * NH
      WRITE (16)         YMDH,GX,GY,NH,(QIJ(I),I=1,N)
      RETURN
      END


      SUBROUTINE PLUMZ(TG,QH,TBAR,STHGT,WS,EFFHT,QP,CIGMX)
C ROUTINE TO COMPUTE EFFECTIVE SOURCE HEIGHT USING BRIGGS PLUME RISE EQS
C INPUTS ARE
C                TG  -  VERTICAL TEMERATURE, GRADIENT, DEG K / METER
C                QH  -  HEAT EMISSION, CAL/SEC
C              TBAR  -  TEMPERATURE, DEG K
C             STHGT  -  STACK HEIGHT, METERS
C                WS  -  WIND SPEED AT STACK HEIGHT, METERS/SEC
C              DIST  -  TRAVEL DISTANCE, METERS
C PLUME RISE IS BASED ON TRAVEL DISTANCE OF FIVE TIMES DISTANCE AT WHICH
C TURBULENCE DOMINATES ENTRAINMENT, I.E. X/X* = 5
      F = 0.000037 * QH
C IF TG IS MISSING OR NON-POSITIVE, USE UNSTABLE OR NEUTRAL FORMULAS
      IF (TG - 999.) 1,4,4
    1 IF (TG + 0.008) 4,4,2
C COMPUTE STABILITY PARAMETER S
    2 THG = TG +0.0098
      S = 9.8 * THG / TBAR
C IF PLUME PENETRATES INVERSION, SET QP = 0
      IF (STHGT - CIGMX) 8,8,3
    3 QP = 0.
    8 CONTINUE
C COMPUTE STABLE PLUME RISE
      DH = 2.9 * (F / (WS * S))**0.33
      GO TO 10
C FIND RAPID RISE DISTANCE X1 FOR NON-STABLE CONDITIONS
    4 IF (STHGT - 305.) 5,5,6
    5 X1 = 2.16 * F**0.4 * STHGT**0.6
      GO TO 7
    6 X1 = 67.3 * F**0.4
C COMPUTE NON-STABLE PLUME RISE
    7 CONTINUE
      XOX1 = 5.
      DH = 1.6 * F**0.33 * X1**0.67 * (0.4 + 0.6*XOX1 + 2.2*XOX1*XOX1)
     1/ (WS * (1. + 0.8*XOX1)**2)
C ADD PLUME RISE TO STACK HEIGHT
   10 EFFHT = STHGT + DH
      RETURN
      END
```

Section 1.0

INTRODUCTION

This appendix presents descriptions, sources and summaries of SO_2 emission, meteorological, and observed SO_2 concentration data for Chicago which were used in the validation analysis of the study presented in the main body of this report. The principal data were obtained on magnetic tape from Argonne National Laboratory and were generated by their APICS data management system (Chamot, et al., 1970). Additional data on source locations and emission inventory results were obtained on punched cards. The data used in the study cover the period 0000 January 1, 1967 to 2300 January 31, 1967. Additional data covering the 13-month period of December 1966 to December 1967 were obtained but not used. A review of these data revealed irregularities in the data and large blocks of missing data. It was assumed that representative judgments could be made from the one-month sample.

Section 2.0

EMISSION DATA

Emission information is available for point sources (the larger emission sources) and a grid work of square areas one mile on a side. Location coordinates of the points and the areas are referenced to fixed coordinates. Information regarding each of these two types of sources is discussed separately in subsequent paragraphs. The development of these data is described in reports from Argonne National Laboratory (Croke, et al., 1968a,b,c; Roberts, et al., 1970; Chamot, et al., 1970).

2.1 AREA SOURCE DATA

For each square mile area an estimate of the annual SO_2 emission rate was obtained for each of three classes of emitters. These include:

Class I: Low rise residential structures consisting of 19 or less dwelling units,

Class II: High rise residential structures, consisting of 20 or more dwelling units, and commercial and institutional buildings, and

Class III: Industrial plants not large enough to be treated as individual point emitters.

In addition to the annual emission rates, estimates regarding effective stack heights and diurnal variations in emission rates were generated in Argonne's extensive study of Chicago emission data. Algorithms for estimating diurnal variations in emission rates are given by Equations (6), (7), and (8) in the Table C-1. In Equations (6) and (7), 20% of the annual emissions are attributed to hot water requirements and distributed evenly over the year. The remaining emissions for Classes I and II are attributed to space heating requirements and are allocated

Table C-1. Chicago Emission Rate Algorithms
(Roberts, et al., 1970; Chamot, et al., 1970)

Utility Source Emission Rate Algortihms**

$$Q_j = 0.1533\ S \sum_{i=1}^{N_i} (w_j)_i\ (A_i L_i + B_i) \qquad (1)$$

Industrial Source Emission Rate Algorithm**

$$Q_j = w_j \left[\left(0.1533\ F_c S_c + 0.1097\ F_o S_o\right)\ \left(U_s U_m L_p + \frac{55-T}{65} L_s\right)\right] \qquad (2)$$

Additional Source Emission Rate Algorithms

(1) Uniform proration

$$Q = \frac{Q_A}{8760^*} \qquad (3)$$

(2) Degree day plus hot water

$$Q = \left[\frac{F_W}{8760} + \frac{(1-F_W)\ (65-T)}{24\ H_D}\right]\ Q_A \qquad (4)$$

(3) Pumping station pattern

$$Q = \frac{U_h Q_A}{8760} \qquad (5)$$

Area Source Emission Rate Algorithms

(1) Residential or commercial low rise

$$Q = \left[\frac{F_W}{8760} + \frac{(1-F_W)\ (65-T-\Delta_R)\ U_h}{D_A H_D}\right]\ Q_A \qquad (6)$$

(continued)

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*8760 hours is one year

**0.1533 = 0.01 (3680)/240, where 3680 = lb SO_2 emitted per ton sulfur in coal, 240 = heat content of coal (therms/ton); 0.1097 = 0.01 (15790)/1440, where 15790 = lb SO_2 emitted per 1000 gal sulfur in oil, 1440 = heat content of oil (therms/1000 gal).

Table C-1. Chicago Emission Rate Algorithms (continued)

(2) Residential or commercial high rise

$$Q = \left[\frac{F_W}{8760} + \frac{(1-F_W)\ (65-T-\Delta_c)}{24D_A} \right] Q_A \qquad (7)$$

(3) Industrial

$$Q = \frac{Q_A}{8760} \qquad (8)$$

Definition of Terms

Q = emission rate, lb/hr

Q_j = emission rate of jth stack in multiple stack source, lb/hr

S = percentage of sulfur in fuel

$(w_j)_i$ = fraction of emissions from ith generating unit going to jth stack

L_i = generating unit output, megawatts

A_i = regression coefficient, therms/megawatt

B_i = regression coefficient, therms

w_j = fraction of emissions going to jth stack

F_c = fraction of fuel requirement filled by coal

F_o = fraction of fuel requirement filled by oil

S_c = percentage of sulfur in coal fuel

S_o = percentage of sulfur in oil fuel

U_s = fraction of average monthly process fuel used during a particular shift (midnight, day or swing on a weekday, Saturday or Sunday (also holiday))

U_m = fraction of maximum process fuel requirement used during mth month

(continued)

Table C-1. Chicago Emission Rate Algorithms (concluded)

L_p = maximum process fuel usage rate, therms/hr

L_s = maximum space heating fuel usage rate, therms/hr

T = temperature, °F

Q_A = annual SO_2 emission, lb/yr

U_h = fraction average hourly fuel usage associated with hth hour

$F_W = 0.2$ = fraction of annual residential/commercial fuel usage attributed to hot water requirements

$D_A = 6155$ = annual degree days, °F day/yr

H_D = hours of fuel usage per day, hr/day

Δ_R = Turner's residential heating temperature correction, °F

Δ_C = Turner's commercial heating temperature correction, °F

U_h Values

(1) Pumping station pattern

$U_h = 0.429$ (hours 0 to 6)

$U_h = 1.29$ (hours 7 to 23)

(2) Area source

$U_h = 1.5$ ($T \leq 5°F$, hours 4 and 5)

($5°F < T < 65°F$, hours 6 and 7)

$U_h = 1.0$ ($T \leq 5°F$, hours 6 to 22)

($5°F < T < 65°F$, hours 8 to 22)

$U_h = 0$ ($T \leq 5°F$, hours 0 to 3 and 23)

($5°F < T < 65°F$, hours 0 to 5 and 23)

($T \geq 65°F$, all hours)

H_D Values

$H_D = 19$ ($T \leq 5°F$)

$H_D = 17$ ($T > 5°F$)

on the basis of outside air temperature deficit below 65°F. Only the first term is applicable in these equations when the outside air temperature is over 65°F. Equation (6) includes a "janitor" factor U_h to account for "hold fire" periods after 10 PM and for a 50% increase in the burn rate during the first two early morning start up hours (starting at 4 AM when temperature is ≤5°F and 6 AM otherwise).

The following effective source heights were used for each class of emitters:

Class	Effective Source Height
I	50 ft
II	200 ft
III	150 ft

The original sources of the area source data were as follows:

Class	Data Source
I	1968 survey by Markets and Rates Dept. of Peoples Gas, Light and Coke (PGLC) Co.
II	1968 (Residential) and 1961 (Commercial) surveys by PGLC Co.
III	1963 survey of annual fuel use by Chicago Dept. of Air Pollution Control

2.2 POINT SOURCES

Point sources are of two types: industrial and power plants. Data relating to power plant emissions include generator operating characteristics, stack heights, location coordinates of the plant site, and the sulfur content of the fuel used. Observed thermal input requirements (fulfilled by burning coal) for observed power output were estimated by Argonne (Roberts, et al.,1970) in the form :

$$T = AL+B$$

where T = thermal input requirement, BTU/hr

L = power output, megawatts

A,B = empirical parameters

The fitted coefficents and the hourly log of power output for the data period were obtained from Argonne. The percentage of the burned fuel exhaust gases diverted to each plant stack (w_j) were obtained for each generator unit. This information is utilized in Equation (1) of the Table C-1 to estimate the emission rate from each stack. The heat content of coal is taken to be 240 therms/ton (a therm is 10^5 BTU's).

The empirical parameters A and B, the fuel sulfur content, the stack height, the plant location coordinates, and the generator-to-stack exhaust coefficients (w_j) are available on punched cards. The hourly power outputs for each generator are available on magnetic tape.

Data relating to the larger industrial emissions treated as point sources include the process operating characteristics and fuel requirements, the plant space heating requirements, the relative amounts of each type fuel used to meet fuel requirements, the sulfur content of each fuel, the percentage of exhaust gas allocated to each plant stack, and the outside air temperature. Fuel requirements for spacing heating were estimated by Argonne to vary from zero at 55°F to a maximum peak value at -10°F. A linear relationship with outside air temperature is assumed to be valid as follows:

$$H_s = \frac{55-T}{65} L_s$$

where H_s = fuel requirements for space heat, therms/hr
T = outside air temperature, °F
L_s = peak space heating requirement, therms/hr

Fuel requirements for industrial processes are related to seasonal and diurnal operating characteristics by means of utilization factors determined from survey questionnaires and interviews with plant operators processed by Argonne (Roberts, et al., 1970). The fuel requirement may be stated as follows:

$$H_p = U_s U_m L_p$$

where H_p = fuel requirement for industrial process, therm/hr
U_s = shift utilization for shift of day (midnight, day or swing) and day of week, fraction of monthly utilization
U_m = month utilization, fraction of peak rate
L_p = peak fuel requirement for industrial processes, therm/hr

All of the above characteristics are reflected in the emission rate algorithm of Equation (2) in Table C-1. Outside air temperatures for the data period are available on magnetic tape. All other data and contained on punched cards. The heat content of coal is taken to be 240 therms/ton. The heat content of oil is taken to be 1440 therms/1000 gal.

Data were also collected regarding certain additional sources which were considered appropriate for treatment as point sources but for which the available data were not compatible with the power plant or industrial emission algorithms. The annual emissions were reported for each source. In addition each source was judged to conform to one of three types of diurnal emission patterns. These patterns consist of uniform emission, hot water plus temperature dependence, and pumping station pattern in which the nighttime emission rate is about one-third the daytime emission rate. The algorithms for estimating emission rates are listed as Equations (3), (4) and (5) in Table C-1. The annual emission rate for each source and its classification by diurnal emission pattern are available on punched cards along with the source location coordinates and stack heights. Emissions are allocated equally among stacks where more than one is present.

Effective stack height was computed using Briggs' (1969) equations for plume rise and the reported stack height for each stack. The heat content of exhaust gases was taken to be 15% of the thermal fuel requirement computed for each source. The amount allocated to each stack is analogous to the emission rate allocated to each stack. In the case of the additional point sources discussed above, an available estimate of the sulfur content of the coal used by each source was used to convert SO_2 emission rates to heat emission rates by the following equation:

$$H_e = 0.15 \frac{240\ Q}{\left(\frac{S}{100}\right) 3680N}$$

where H_e = heat emission rate, therms/hr

Q = SO_2 emission rate, lb/hr

S = fuel sulfur content, percent

N = number of stacks

The numbers 240 and 3680 represent the therms per ton of coal and the pounds of SO_2 emitted per ton of sulfur in burned fuel, respectively. The number 0.15 is the fraction of coal heat content contained in the exhaust gases.

Section 3.0

METEOROLOGICAL DATA

The meteorological data for Chicago which are required for the validation analysis include wind speed and direction, temperature, cloud cover and types, cloud heights and ceiling, and the height of the top of the mixing layer. Three types of data were utilized. These include TAM (Telemetered Air Monitoring) Station wind data, Midway Airport hourly airway observations and hourly estimates of the top of the mixing layer.

An average wind speed and direction based on continuous measurements over a 75-minute period centered on each hour was available for each TAM site. The anemometer and wind vane height at these stations was generally above building heights and varied from 40 feet to 180 feet; the average height was 80 feet. A vector average of the observations for each hour was used to determine the mean wind speed and direction for the validation study.

The Midway Airport observations were used to get the outside air temperature for making temperature dependent emission estimates and for determining stability classifications by means of the Turner (1964) classification scheme.

Argonne had obtained hourly estimates of the top of the mixing layer using Midway surface temperatures and rural vertical temperature profiles. The rural vertical temperature profile was constructed using Green Bay and Peoria radiosonde data for 0600 and 1800 CST and the

Argonne surface temperature. An interpolation between the two soundings was made to fit the Argonne surface temperature if appropriate. Otherwise, one sounding or the other was shifted to fit to the Argonne temperature. Linear interpolations were made for hourly intervals between the 12-hour observation periods. The mixing layer ceiling was estimated by the intersection of the Midway potential temperature with rural temperature profile.

Section 4.0

SO_2 OBSERVATIONS

Mean hourly concentrations of SO_2 at each of eight TAM stations were obtained on magnetic tape for the data period.

Concentrations measured by TAM station analyzers and averaged over 24-hour periods were compared with 24-hour concentrations measured by the West-Gaeke method (Booras and Zimmer 1968). The West-Gaeke method averaged about 20% lower than the conductivity method. However. as shown in the 2-hour versus 24-hour comparisons for St. Louis (Appendix B), this could be due to the use of 24-hour samples in the West-Gaeke method. The methods showed large deviations in both directions (either one high relative to the other). Interference from other pollutants was clearly evident at certain locations (e.g., TAM Station #3 in the Chicago Loop area) where the mean concentration measured by conductivity was twice that measured by the West-Gaeke method. As a result of this analysis and those reported by other investigators (e.g., Shikiya and MacPhee 1969), it is seen that observed concentrations for single steady-state periods may be in error by a factor of two.

Section 5.0

CHICAGO PREPROCESSING PROGRAM LISTINGS

```fortran
C CHICAGO DATA PREPROCESSOR
      DIMENSION XP(200),YP(200),HP(200),NS(30),SPCT( 30),QPTOT( 30),
     1NPAT( 30),HGTI(4,100),COALP(100),OILP(100),SPCIC(100),SPCIO(100)
     2,XR(10),YR(10),ZR(10),HA(5),ZP(200),WDAY(7,100),P(5),QH(200)
      DIMENSION STKPI(4,100),PMUF(12,100),SFWP(9,100),SPHTG(100),QP(200)
      DIMENSION HGTU(6,6),NSU(6),NUNIT(6),SPCTU(6),STKPU(24,6),A(4,6)
     1,B(4,6),ULOAD(4,6),QHU(6),QPU(6),QPS(6)
      DIMENSION PROCL(100),OBCON(10),QPI(4),QHI(4),EFHGT(6),UDH(200)
      DATA NADPT/27/
      DATA NINPT/52/
      DATA NUTPT/6/
      DATA NRECP/8/
      DATA XR/5.3,10.5,13.3,14.4,11.1,12.7,6.7,7.9/
      DATA YR/25.6,10.7,17.9,11.6,11.7,5.3,18.8,9.3/
      DATA ZR/8*0./
      DATA GX/20./
      DATA GY/30./
      DATA DLTA/1609.3/
      DATA NH/3/
C HA IS HEIGHT OF AREA SOURCES IN METERS
      DATA HA/30.5,45.7,61./
      DATA Z1/20./
      DATA P/0.1,0.1,0.15,0.2,0.3/
      DATA ICARD/5/
      DATA IPRTR/6/
      READ (ICARD,1003) IREC1,NREC
 1003 FORMAT (2I5)
C GET POINT SOURCE EMISSION PARAMETERS
      CALL INC1(NADPT,XP,YP,HP,NS ,SPCT,QPTOT,NPAT,IPRTR)
      N1 = NADPT
      CALL INC2(N1,NINPT,XP,YP,WDAY,HGTI,COALP,OILP,SPCIC,SPCIO,STKPI
     1,PMUF,SFWP,SPHTG,PROCL,IPRTR)
      N1 = N1 + NINPT
      CALL INC3(N1,NUTPT,XP,YP,HGTU,NSU,NUNIT,SPCTU,STKPU,A,B,IPRTR)
      II = IREC1 - 1
      IF (II) 2,2,1
    1 CONTINUE
      DO 3 I=1,II
      READ (16)
      READ (17)
    3 CONTINUE
    2 CONTINUE
      DO 400 I1=1,NREC
      IR = I1
      CALL INC4(CY,CM,CD,CH,DOW,THTA,U1,TEMP,CEIL,PRES,CSUM4,TUNC,CIGMX
     1,OBCON,IR)
      TBAR = (TEMP - 32.) * 1.8 + 273.
      IF (TUNC - 5.) 6,5,4
    4 CONTINUE
      WRITE(IPRTR,1000) TUNC
 1000 FORMAT(' STABILITY PARAMETER IS OUT OF RANGE, TUNC =',F6.1)
    5 CONTINUE
      TG = -0.0065
      GO TO 7
    6 CONTINUE
      TG = 999.
    7 CONTINUE
      INDEX = TUNC
      PWIND = P(INDEX)
      CALL INC5(CYY,CMM,CDD,CHH,DOWW,NUTPT,NUNIT,ULOAD,IR)
C CHECK DATE/TIME DATA
      IF (CY - CYY) 10,20,10
   10 CONTINUE
      WRITE (IPRTR,1001) CY,CM,CD,CH,DOW,CYY,CMM,CDD,CHH,DOWW
 1001 FORMAT(' DATE/TIME DATA FROM MET AND LOAD FILES DISAGREE     YEAR
     1 MONTH      DAY     HOUR WEEKDAY'/40X'MET FILE',5F8.0/39X'LOAD FILE'
     2,5F8.0)
      CALL EXIT
   20 CONTINUE
      IF (CM - CMM) 10,30,10
   30 CONTINUE
      IF (CD - CDD) 10,40,10
   40 CONTINUE
      IF (CH - CHH) 10,50,10
   50 CONTINUE
      IF (DOW - DOWW) 10,60,10
   60 CONTINUE
      M = CM
C COMPUTE EMISSION RATE AND EFFECTIVE HEIGHT FOR ADDITIONAL POINTS
      DO 100 I2=1,NADPT
      CALL APSHE(TEMP,SPCT(I2),QPTOT(I2),NPAT(I2),NS(I2),CH,QP(I2)
     1,QH(I2))
      WS = U1 * (HP(I2) / Z1)**PWIND
      IF (QH(I2)) 70,70,80
   70 CONTINUE
      ZP(I2) = HP(I2)
      GO TO 90
   80 CONTINUE
      CALL PLUMZ(TG,QH(I2),TBAR,HP(I2),WS,ZP(I2),QP(I2),CIGMX)
   90 CONTINUE
      UDH(I2) = WS * (ZP(I2) - HP(I2))
  100 CONTINUE
C COMPUTE EMISSION RATE AND EFFECTIVE HEIGHT FOR INDUSTRIAL POINTS
      DO 200 I3=1,NINPT
C GET SHIFT AND WEEKDAY INDEXES
      IF (DOW - 7.) 110,110,105
  105 CONTINUE
      ID = 3
      GO TO 115
  110 CONTINUE
      IDW = DOW
      ID    = WDAY(IDW,I3)
  115 CONTINUE
      CALL SHFTC(HOUR,IS)
      CALL IPSHE(SPHTG(I3),PROCL(I3),TEMP,COALP(I3),OILP(I3),SPCIC(I3)
     1,SPCIO(I3),STKPI(1,I3),PMUF(1,I3),SFWP(1,I3),M,IS,ID,QPI,QHI)
      NI = NADPT + I3
      QP(NI) = 0
      ZP(NI) = 0
      QH(NI) = 0
      HP(NI) = 0
      UDH(NI) = 0
      DO 140 I=1,4
      IF (HGTI(I,I3)) 140,140,120
  120 CONTINUE
      IF (QHI(I)) 140,140,130
  130 CONTINUE
      WS = U1 * (HGTI(I,I3) / Z1)**PWIND
      CALL PLUMZ(TG,QHI(I),TBAR,HGTI(I,I3),WS,EFHGT(I),QPI(I),CIGMX)
      QP(NI) = QP(NI) + QPI(I)
      QH(NI) = QH(NI) + STKPI(I,I3) * QHI(I)
      HP(NI) = HP(NI) + STKPI(I,I3) * HGTI(I,I3)
      UDH(NI) = UDH(NI) + STKPI(I,I3) * WS * (EFHGT(I) - HGTI(I,I3))
      ZP(NI) = ZP(NI) + STKPI(I,I3) * EFHGT(I)
  140 CONTINUE
  200 CONTINUE
C COMPUTE EMISSION RATE AND EFFECTIVE HEIGHT FOR UTILITY POINT SOURCES
      N1 = NI
      DO 300 I4=1,NUTPT
      CALL UPSHE(NSU(I4),NUNIT(I4),SPCTU(I4),            STKPU(1,I4)
     1,A(1,I4),B(1,I4),ULOAD(1,I4),QHU,QPU,QPS)
      NI = N1 + I4
      QP(NI) = 0
      ZP(NI) = 0
      QH(NI) = 0
      HP(NI) = 0
      UDH(NI) = 0
      II = NSU(I4)
      DO 240 I=1,II
      IF (QHU(I)) 240,240,230
  230 CONTINUE
      WS = U1 * (HGTU(I,I4) / Z1)**PWIND
      CALL PLUMZ(TG,QHU(I),TBAR,HGTU(I,I4),WS,EFHGT(I),QPS(I),CIGMX)
      QP(NI) = QP(NI) + QPS(I)
      QH(NI) = QH(NI) + QHU(I)
  240 CONTINUE
      QH(NI) = QH(NI) / II
      IF (QP(NI)) 300,300,244
  244 CONTINUE
      DO 250 I=1,II
      EHW = QPS(I) / QP(NI)
      ZP(NI) = ZP(NI) + EHW * EFHGT(I)
      HP(NI) = HP(NI) + EHW * HGTU(I,I4)
      UDH(NI) = UDH(NI) + EHW * (EFHGT(I) - HGTU(I,I4))
  250 CONTINUE
  300 CONTINUE
      NRPNT =NI
C WRITE OUTPUT RECORD
      CALL OUTC(CY,CM,CD,CH,DOW,NRECP,XR,YR,ZR,GX,GY,DLTA,NH,HA,NRPNT,XP
     1,YP,ZP,QP,U1,Z1,PWIND,THTA,INDEX,CIGMX,TEMP,OBCON,IR,XNDX,PRES)
      IF (CH - 23.) 320,310,320
  310 CONTINUE
      WRITE (IPRTR,1002) XNDX
 1002 FORMAT(' RECORD, WITH INDEX =',F10.0,', WRITTEN ON UNIT 19')
  320 CONTINUE
  400 CONTINUE
      END FILE 19
      REWIND 12
      REWIND 13
      REWIND 14
      REWIND 16
      REWIND 17
      REWIND 19
      CALL EXIT
      END



      SUBROUTINE INC1(NADPT,XP,YP,ZP,NS,SPCT,QPTOT,NPAT,IPRTR)
      DIMENSION XP(1),YP(1),ZP(1),NS(1),SPCT(1),QPTOT(1),NPAT(1)
      DO 100 I=1,NADPT
      READ(    12    ) J,XP(I),YP(I),ZP(I),NS(I),SPCT(I),QPTOT(I),NPAT(I)
      IF (J - I) 10,20,10
   10 CONTINUE
      WRITE(IPRTR,1000) I,J
 1000 FORMAT(' ORDER ERROR DETECTED READING RECORD NO.',I6,', RECORD NO.
     1ON FILE WAS',I6,' (INC1)')
      CALL EXIT
   20 CONTINUE
      IF(NS(I)) 425,425,450
  425 CONTINUE
      NS(I) = 1
  450 CONTINUE
C CONVERT STACK HEIGHTS FROM FT TO M
      ZP(I) = 0.3048 * ZP(I)
  100 CONTINUE
      RETURN
      END
      SUBROUTINE INC2(N1,NINPT,XP,YP,A,  H,COALP,OILP,SPCTC,SPCTO,STAKP
     1,PMUF,SFWP,SPHTG,PROCL,IPRTR)
      DIMENSION XP(1),YP(1),      H(4,1),CCALP(1),OILP(1),SPCTC(1),A(7,1)
     1,SPCTO(1),STAKP(4,1),PMUF(12,1),SFWP(9-1),SPHTG(1),PROCL(1)
      I = N1
      DO 100 J=1,NINPT
      I = I + 1
      READ(  13  )K,XP(I),YP(I),(H(L,J),STAKP(L,J),L=1,4),(A(L,J),L=1,7)
     1,SPHTG(J),PRCCL(J),(PMUF(L,J),L=1,12),(SFWP(L,J),L=1,9),SPCTC(J)
     2,COALP(J),SPCTO(J),OILP(J)
      IF (J - K) 10,20,10
   10 CONTINUE
      WRITE (IPRTR,1000) J,K
 1000 FORMAT(' ORDER ERROR DETECTED READING RECORD NO.',I6,', RECORD NO.
     1ON FILE WAS',I6,' (INC2)')
      CALL EXIT
   20 CONTINUE
      DO 30 L=1,4
C CONVERT STACK HEIGHTS FROM FT TO M
      H(L,J) = 0.3048 * H(L,J)
C CONVERT STAKP TO FRACTION
      STAKP(L,J) = STAKP(L,J) / 100.
   30 CONTINUE
C CONVERT COALP AND OILP TO FRACTION
      COALP(J) = COALP(J) * .01
      OILP(J) = .01 * OILP(J)
C CONVERT PUMF TO FRACTION
      DO 200 L=1,12
      PMUF(L,J) = PMUF(L,J) * .1
 200  CONTINUE
C CONVERT SFWP TO FRACTION
      DO 250 L=1,9
      SFWP(L,J)=SFWP(L,J)*.01
 250  CONTINUE
  100 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE INC3(N1,NUTPT,XP,YP,HGTU,NSU,NUNIT,SPCTU,STKPU,A,B
     1,IPRTR)
      DIMENSION XP(1),YP(1),          NSU(1),NUNIT(1),SPCTU(1),STKPU(24,1)
     1,A(4,1),B(4,1),HGTU(6,1)
      I = N1
      DO 100 J=1,NUTPT
      I = I + 1
      READ(   14   ) K,XP(I),YP(I),NSU(J),(HGTU(L,J),L=1,6),NUNIT(J)
     1,SPCTU(J),(STKPU(L,J),L=1,24),(A(L,J),L=1,4),(B(L,J),L=1,4)
      IF (J - K) 10,20,10
   10 CONTINUE
      WRITE (IPRTR,1000) J,K
 1000 FORMAT(' ORDER ERROR DETECTED READING RECORD NO.',I6,', RECORD NO.
     1ON FILE WAS',I6,' (INC3)')
      CALL EXIT
   20 CONTINUE
C CONVERT STACK HEIGHTS FROM FT TO M
      DO 30 L=1,6
      HGTU(L,J) = 0.3048 * HGTU(L,J)
   30 CONTINUE
C CONVERT STAKP TO A FRACTION
      DO 50 L=1,24
      STKPU(L,J)=STKPU(L,J)*.01
 50   CONTINUE
  100 CONTINUE
      RETURN
      END
      SUBROUTINE INC4(CY,CM,CD,CH,DOW,  WD,U1,TEMP,CEIL,PRES,CSUM4,TUNC
     1,CIGMX,OBCON,IR)
      DIMENSION OBCON(1)
      READ(    16    ) I,U1,WD,TEMP,CEIL,PRES,CSUM4,TUNC,CIGMX,(OBCON(K),
     1K=1,8),CH,DOW,CD,CM,CY
      RETURN
      END


      SUBROUTINE INC5(CYY,CMM,CDD,CHH,DOWW,NUTPT,NUNIT,ULOAD,IR)
      DIMENSION NUNIT(1),ULOAD(4,1),ALOAD(20)
      READ(    17    )I,CYY,CMM,CDD,DOWW,CHH,(ALOAD(J),J=1,15)
      K = 0
      DO 20 I=1,NUTPT
      JJ = NUNIT(I)
      DO 10 J=1,JJ
      K = K + 1
      ULOAD(J,I) = ALOAD(K)
   10 CONTINUE
   20 CONTINUE
      RETURN
      END


      SUBROUTINE PLUMZ(TG,QH,TBAR,STHGT,WS,EFFHT,QP,CIGMX)
C ROUTINE TO COMPUTE EFFECTIVE SOURCE HEIGHT USING BRIGGS PLUME RISE EQS
C INPUTS ARE
C                   TG   -  VERTICAL TEMERATURE, GRADIENT, DEG K / METER
C                   QH   -  HEAT EMISSION, CAL/SEC
C                 TBAR   -  TEMPERATURE, DEG K
C                STHGT   -  STACK HEIGHT, METERS
C                   WS   -  WIND SPEED AT STACK HEIGHT, METERS/SEC
C                 DIST   -  TRAVEL DISTANCE, METERS
C PLUME RISE IS BASED ON TRAVEL DISTANCE OF FIVE TIMES DISTANCE AT WHICH
C TURBULENCE DOMINATES ENTRAINMENT, I.E. X/X* = 5
      F = 0.000037 * QH
C IF TG IS MISSING OR NON-POSITIVE, USE UNSTABLE OR NEUTRAL FORMULAS
      IF (TG - 999.) 1,4,4
    1  IF (TG + 0.008)4,4,2
C COMPUTE STABILITY PARAMETER S
    2 THG = TG +0.0098
      S = 9.8 * THG / TBAR
C IF STACK HEIGHT EXCEEDS MIXING CEILING, SET QP = 0
      IF (STHGT - CIGMX) 8,8,3
    3 QP = 0.
    8 CONTINUE
C COMPUTE STABLE PLUME RISE
      DH = 2.9 * (F / (WS * S))**0.33
      GO TO 10
C FIND RAPID RISE DISTANCE X1 FOR NON-STABLE CONDITIONS
    4 IF (STHGT - 305.) 5,5,6
    5 X1 = 2.16 * F**0.4 * STHGT**0.6
      GO TO 7
    6 X1 = 67.3 * F**0.4
C COMPUTE NON-STABLE PLUME RISE
    7 CONTINUE
      XOX1 = 5.
      DH = 1.6 * F**0.33 * X1**0.67 * (0.4 + 0.6*XOX1 + 2.2*XOX1*XOX1)
     1/ (WS * (1. + 0.8*XOX1)**2)
C ADD PLUME RISE TO STACK HEIGHT
   10 EFFHT = STHGT + DH
      RETURN
      END
      SUBROUTINE APSHE(TEMP,SULPC,QPTOT,NPAT,NS,HR,QAPHR,QHEAT)
C INPUTS
C           TEMP       TEMPERATURE (DEG F)
C           SULPC      SULFUR CONTENT OF FUEL (PERCENT)
C           QPTOT      ANNUAL EMISSION OF SO2    00 LB/YR)
C           NPAT       EMISSION PATTERN - 1=UNIFORM,2=TEMP DEPENDENT,3=PUMP
C           NS         NUMBER OF STACKS
C           HR         HOUR OF DAY
C OUTPUTS
C           QAPHR      SO2  EMISSION RATE (G/SEC)
C           QHEAT      HEAT EMISSION RATE (CAL/SEC)
C CHEAT CONVERTS  (      THERMS/HR) TO (CAL/SEC)
      DATA CHEAT/7.000E3/
C THTON IS COAL HEAT CONTENT (      THERMS/TON)
      DATA THTON/240./
C SO2SU IS SO2 EMISSION FACTOR FOR SULFUR IN COAL (LB SO2/TON SULFUR)
      DATA SO2SU/3680./
C CRATE CONVERTS LB/HR TO G/SEC
      DATA CRATE/0.1260/
C DEGDA IS ANNUAL DEGREE DAYS
      DATA DEGDA/6155./
C DETERMINE METHOD OF CALCULATION FOR EMISSION PATTERN
      GO TO (100,200,300),NPAT
  100 CONTINUE
C UNIFORM EMISSION
      QAPHR=QPTOT/8760.
      GO TO 400
  200 CONTINUE
C TEMP DEPENDENT EMISSION
      IF(TEMP-65) 250,225,225
  225 CONTINUE
      TE=0.
      GO TO 275
  250 CONTINUE
      TE=1.
  275 CONTINUE
      QAPHR=QPTOT*(.2/(8760.) + .8*TE*(65.-TEMP )/(24. * DEGDA))
      GO TO 400
C PUMP STATION PATTERN
  300 CONTINUE
      TPUMP=.429
      IF(6.9-HR) 350,375,375
  350 CONTINUE
      IF(HR-23.1) 370,375,375
  370 CONTINUE
C HOUR IS LT 23.1 AND GT 6.9
      TPUMP=1.29
  375 CONTINUE
      QAPHR= QPTOT*TPUMP/8760.
  400 CONTINUE
C CALCULATE HEAT EMISSION FOR SINGLE STACK SIMULATION OF MULTIPLE STACKS
C ASSUMPTIONS-
C                 - STACK HEIGHTS ARE EQUAL
C                 - SO2 AND HEAT DISTRIBUTION AMONG STACKS IS UNIFORM
C                 - COAL IS USE AS A FUEL
      QHEAT = (QAPHR * THTON) / (0.01 * SULPC * SO2SU *  NS)
      QHEAT = QHEAT * CHEAT

C QA IS IN UNITS OF LBS/HR CONVERT TO GRAMS/SEC
      QAPHR = CRATE * QAPHR
      RETURN
      END
      SUBROUTINE IPSHE(SPHTG,PROCL,TEMP,COALP,OILP,SULPC,SULPO,STAKP,
     CPMUF,SFWP,M,IS,ID, QSO2S,QTSTK)
C IPSHE CALCULATES THE HOURLY EMISSION FROM INDUSTRIAL POINT SOURCES
C INPUTS
C           SPHTG      MAX. SPACE HEATING REQD. (THERMS/HR)
C           PROCL      MAX. PROCESS LOAD (THERMS/HR)
C           TEMP       TEMPERATURE (DEG F)
C           COALP      COAL LOAD (FRACTION)
C           OILP       OIL LOAD (FRACTION)
C           SULPC      SULFUR CONTENT OF COAL (PERCENT)
C           SULPO      SULFUR CONTENT OF OIL (PERCENT)
C           STAKP      STACK EMISSION ALLOCATION (FRACTION)
C           PMUF       MONTH EMISSION ALLOCATION (FRACTION)
C           SFWP       SHIFT EMISSION ALLOCATION (FRACTION)
C           M          MONTH OF YEAR INDEX
C           IS         SHIFT INDEX (1=1-8, 2=9-16, 3=17-24)
C           ID         DAY OF WEEK INDEX (1=WEEKDAY,2=SAT,3=SUN OR HOLIDAY)
C OUTPUTS
C           QSO2S      SO2  EMISSION RATE (G/SEC)
C           QTSTK      HEAT EMISSION RATE (CAL/SEC)
      REAL LS,LP,L,LC,LO
      DIMENSION PMUF(12),SFWP(3,3),STAKP(4),QSO2S(4),QTSTK(4)
C HEATC IS COAL HEAT CONTENT (THERMS/TON)
      DATA HEATC/240./
C HEATO IS OIL HEAT CONTENT (THERMS/1000 GAL)
      DATA HEATO/1440./
C SO2CO IS SO2 EMISSION FACTOR FOR SULFUR IN COAL (LB SO2/TON SULFUR)
      DATA SO2CO/3680./
C SO2OI IS SO2 EMISSION FACTOR FOR SULFUR IN OIL (LB SO2/1000 GAL SULFR)
      DATA SO2OI/15790./
C HEATE IS HEAT LOSS TO FLUE GASES (FRACTION)
      DATA HEATE/0.15/
C CHEAT CONVERTS THERMS/HR TO CAL/SEC
      DATA CHEAT/7.000E3/
C CRATE CONVERTS LB/HR TO G/SEC
      DATA CRATE/0.1260/
      IF (TEMP - 55.) 10,10,20
   10 CONTINUE
      LS = 0.
      GO TO 30
   20 CONTINUE
      LS = SPHTG*(55.-TEMP)/65.
   30 CONTINUE
      LP = PROCL*PMUF(M)*SFWP(IS,ID)
C LS AND LP ARE THE ADJUSTED HEATING AND PROCESS LOADS

      L = LP+LS
C L IS TOTAL LOAD
      LC = COALP*L
      LO = OILP*L
C LC AND LO ARE COAL AND OIL LOADS

      C = LC / HEATC
C C IS THE HOURLY RATE OF COAL USE
      O = LO / HEATO
C O IS THE HOURLY RATE OF OIL USE
      QC = 0.01 * SULPC * C * SO2CO
      QS = 0.01 * SULPO * O * SO2OI
C QC AND QS ARE SO2 EMISSION RATES FOR COAL AND OIL
      QSO2 = (QC + QS) * CRATE
C ALLOCATE SO2 EMISSION AND THERMAL OUTPUT TO STACKS
      DO 300 I=1,4
      QSO2S(I)= STAKP(I)*QSO2
      QTSTK(I) = STAKP(I) * HEATE * L * CHEAT

  300 CONTINUE
      RETURN
      END
      SUBROUTINE UPSHE(NSTAK,NUNIT,SULPC,       STAKP,A,B,XL,THOSK,SO2UN,
     CSO2SK)
C     CALCULATE UTILITY POINT  SOURCE HOURLY EMISSIONS
C  INPUTS
C          NSTAK      NO. OF STACKS
C          NUNIT      NO. OF GENERATOR UNITS
C          SULFC      SULFUR CONTENT OF COAL (PERCENT)
C          STAKP      STACK EMISSION ALLOCATION BY GEN. UNIT (FRACTION)
C          A          REGRESSION COEF (THERMAL LOAD ON POWER OUTPUT),SLOPE
C          B          REGRESSION COEF ,INTERCEPT
C          XL         POWER OUTPUT (MEGAWATTS)
C  OUTPUTS
C          THOSK      HEAT EMISSION RATE
C          SO2UN      SO2  EMISSION RATE BY GEN. UNIT
C          SO2SK      SO2  EMISSION RATE BY STACK
      DIMENSION THIUN(4)          ,STAKP(6,4),THOUN(4),THOSK(6),SO2UN(4),
     CSO2SK(6),A(4),B(4),XL(4)
C HEATE IS HEAT LOSS TO FLUE GASES (FRACTION)
      DATA HEATE/0.15/
C HEATC IS COAL HEAT CONTENT (THERMS/TON)
      DATA HEATC/240./
C SO2CO IS SO2 EMISSION FACTOR FOR SULFUR IN COAL (LB SO2/TON SULFUR)
      DATA SO2CO/3680./
C CHEAT CONVERTS THERMS/HR TO CAL/SEC
      DATA CHEAT/7000./
C CRATE CONVERTS LB/HR TO G/SEC
      DATA CRATE/0.1260/

      DO 30 K=1,NUNIT
C CALCULATE THERMAL LOADS FOR EACH UNIT
      THIUN(K)=A(K)*XL(K)+B(K)
      IF (THIUN(K)) 20,25,25
   20 CONTINUE
      THIUN(K) = 0.
   25 CONTINUE
      THOUN(K) = HEATE * THIUN(K)
C CALCULATE SO2 EMISSION FROM K TH UNIT
      C = THIUN(K) / HEATC
      SO2UN(K) = 0.01 * SULPC * C * SO2CO
 30   CONTINUE
      DO 100 I=1,NSTAK
      SO2SK(I)=0.
      THOSK(I)=0.
 100  CONTINUE
C START STACK ALOCATION LOOP
      DO 200 J=1,NSTAK
      DO 200 K=1,NUNIT
      SO2SK(J)=STAKP(J,K)*SO2UN(K) + SO2SK(J)
 200  CONTINUE
C SO2SK IS IN UNITS OF LBS/HR - CONVERT TO GRAMS / SEC
      DO 400 J=1,NSTAK
      SO2SK(J) = CRATE * SO2SK(J)
      DO 300 K=1,NUNIT
      THOSK(J)= STAKP(J,K)*THOUN(K)+THOSK(J)
 300  CONTINUE
      THOSK(J) = THOSK(J) * CHEAT
  400 CONTINUE
      RETURN
      END
      SUBROUTINE SHFTC(HOUR,IS)
C DETERMINE SHIFT
      IF (HOUR) 13,13,9
    9 CONTINUE
      IF (HOUR - 17.) 10,13,13
   10 CONTINUE
      IF (HOUR - 9.) 11,12,12
C MIDNIGHT SHIFT (01 - 08)
   11 CONTINUE
      IS = 1
      GO TO 14
C DAY SHIFT (09 - 16)
   12 CONTINUE
      IS = 2
      GO TO 14
C SWING SHIFT (17 - 24)
   13 CONTINUE
      IS = 3
   14 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE OUTC(CY,CM,CD,CH,DOW,NRECP,XR,YR,ZR,GX,GY,DLTA,NH,HA
     1,NRPNT,XP,YP,ZP,QP,WS,WH,P,WD,INDEX,CIGMX,TEMP,OBS,IR,XNDX,STAPR)
      DIMENSION XR(1),YR(1),ZR(1),HA(1)       ,XP(1),YP(1),ZP(1),QP(1)
     1,OBS(1)
C COMPUTE RECORD INDEX NUMBER
      XNDX = CH + 100. * CD + 1.E4 * CM
C SET OTHER PARAMETER VALUES
      IDOW = DOW
      SIGA = 0.
      RIB = 0.
      PCPN = 0.
      WGLD = 0.
      WRITE (     19     ) XNDX,CY,CM,CD,IDOW,CH,NRECP,(XR(I),I=1,NRECP)
     1,(YR(I),I=1,NRECP),(ZR(I),I=1,NRECP),(OBS(I),I=1,NRECP),GX,GY,DLTA
     2,NH,(HA(I),I=1,NH),NRPNT,(XP(I),I=1,NRPNT),(YP(I),I=1,NRPNT)
     3,(ZP(I),I=1,NRPNT),(QP(I),I=1,NRPNT),WS,WH,P,WD,INDEX,TEMP,CIGMX
     4,SIGA,RIB,PCPN,WGLD,STAPR
      RETURN
      END
```

Exhibit D-1

LISTING OF FORTRAN CODE COMPUTER PROGRAM AND SUBROUTINES USED FOR VALIDATION CALCULATIONS*

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*Additional subroutines are listed in Exhibit D-3.

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C DIFFUS2
C MAIN PROGRAM FOR VALIDATION CALCULATIONS
      DIMENSION YEARR(2),AMONN(2),DAYY(2),HOURR(2)
      DIMENSICN CNCT(50),CAREA(50),CPCIN(50),XRR(50),YRR(50)
     1,ZRR(50),OBSO2(50)
      DIMENSION DISTX(1000),XDCAY(2000),SSIGZ(1000),EXPOZ(2000)
     1,HA(5),UHA(5),QXY(5),Q(4000)
      DIMENSION XP (100),YP (100),ZP (100),QP(100)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/DATIME /DH,STOP,YEARR,AMONN,DAYY,HOURR,HOURL
      COMMON/OUTPUT/YEAR,AMON,DAY,HOUR ,NRECP,CNCT,CAREA,CPCIN
     1,XRR,YRR,ZRR,OBSO2,IDUW,NR1,TEMP,SIGA,RIB,PCPN,WGLD,STAPR
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,NH,HA
      1,UHA,QXY,Q,CONC,NH1
      COMMON/WNDSP/WSPD,WHGT,PWIND
      COMMON/POINTS/NPS   ,XP  ,YP  ,ZP  ,QP,CONPS,NPSS
C NXLIM GIVES DIMENSION LIMIT OF DISTX AND SSIGZ ARRAYS.
C NXZLM DEFINES DIMENSION LIMIT OF EXPOZ AND XDCAY ARRAYS
C NNH  DEFINES DIMENSION LIMIT OF UHA AMD HA ARRAYS
C NR   DEFINES DIMENSION LIMIT OF XRR, YRR, ZRR AND CNCT ARRAYS.
C NNPS DEFINES DIMENSION LIMIT OF XP , YP , ZP  AND QP ARRAYS.
C NA   DEFINES DIMENSION LIMIT OF Q ARRAY.
      DATA NR/50/
      DATA NNH/5/
      DATA NNPS/100/
      DATA NA/4000/
      NXLIM = 1000
      NXZLM = 2000
      HOURL = 24.
C     HOURL = 23.
C GET CONTROL PARAMETERS
      CALL PRAMB
      IF (ISIGD) 2,2,3
    2 CONTINUE
      WRITE (IPRTR,1007) ISIGD
 1007 FORMAT (' ISIGD OUT OF RANGE =',I5)
      CALL EXIT
    3 CONTINUE
      IF (ISIGD - 4) 4,4,2
    4 CONTINUE
      WRITE (IPRTR,1008) NLI,ISIGD,XONE,CONX,      DECAY
 1008 FORMAT ('1CONTROL PARAMETERS FOR THIS CONTR MODEL RUN'
     1,5X'NLI    ISIGD     XONE       CONX    DECAY'/44X2I8,F8.1
     2,F8.3///)
      READ(ICARD,1000)(YEARR(I),AMONN(I),DAYY(I),HOURR(I),I=1,2),DH
 1000 FORMAT (1X ,8(3X,F2.0),F5.0)
      WRITE(IPRTR,1009)DH,(YEARR(I),AMONN(I),DAYY(I),HOURR(I),I=1,2)
 1009 FORMAT (' RANGE OF DATES IN DATA SETS REQUESTED, HOUR'
     1,' INCREMENT IN REQUESTS =',F5.0//'   YEAR MONTH   DAY'
     2,' HOUR'/1X4F6.0/1X4F6.0)
   20 CONTINUE
C GET DATA FOR ONE STEADY STATE PERIOD
      YEAR = YEARR(1)
      AMON = AMONN(1)
      DAY = DAYY(1)
      HOUR = HOURR(1)
      CALL DAFIL
C     CALL CHIDA
C DETERMINE THAT DATA HAS NOT OVERFLOWED PROGRAM LIMITS AND
C THAT DIMENSION LIMITS ARE NOT VIOLATED.
      IF (NRECP - NR) 22,22,21
   21 CONTINUE
      WRITE (IPRTR,1006) GX,GY,NRECP,NH,NPS
 1006 FORMAT (' PROGRAM DIMENSION LIMITS EXCEEDED.      GX'
     1,7X'GY    NRECP',6X'NH       NPS'/35X2F8.0,3I8/' SKIP TO'
     2,' NEXT DATA SET')
```

```
      GO TO 160
   22 CONTINUE
      IF(NPS-NNPS) 23,23,21
   23 CONTINUE
      NGV = GX * GY * NH
      IF (NGV - NA) 24,24,21
   24 CONTINUE
      IF(NH-NNH) 28,28,27
   27 CONTINUE
      WRITE (IPRTR,1005) NNH,NH
 1005 FORMAT('NH EXCEEDS DIMENSION LIMIT OF',I4,',NH=',I4
     1,'NH SET TO LIMIT')
      NH=NNH
   28 CONTINUE
      AREA = DLTA * DLTA
      DO 29 IG=1,NGV
      Q(IG) = Q(IG) / AREA
   29 CONTINUE
      NPSS = NPS
      XYMIN = 0.5 * DLTA
      XSMAX = (GX + 0.5) * DLTA
      YSMAX = (GY + 0.5) * DLTA
C CHECK VALIDITY OF WIND DATA, SKIP TO NEXT DATA SET IF WIND
C SPEED LIES OUTSIDE 0 TO 30 OR WIND DIRECTION LIES OUTSIDE
C -PI/2 TO 2.5*PI
      IF (WSPD - 1.) 150,150,30
   30 CONTINUE
      IF (WSPD - 30.) 31,150,150
   31 CONTINUE
      IF (THTA - 7.9) 40, 40,150
   40 CONTINUE
      IF (THTA + 1.6) 150,150,41
   41 CONTINUE
C SET COS AND SIN FACTORS FOR WIND/SOURCE COORDINATE CONVERSIONS
      ISTAR = 0
      CALL SCORD
      CALL WCORD
      CALL SIGZZ
      IF (IERR) 50,45,50
   45 CONTINUE
      ISTAR = 1
      CALL DISTB
      IF (IERR) 60,60,50
   50 CONTINUE
      WRITE (IPRTR,1001) YEAR,AMON,DAY,HOUR
 1001 FORMAT (' INPUT ERROR, GO TO NEXT DATA SET',4F8.0)
      GO TO 160
   60 CONTINUE
C GET CONCENTRATION FOR EACH RECEPTOR LOCATION
      ZR = -1
C     NRECP = 10
      DO 140 I=1,NRECP
      XR=XRR(I) * DLTA
C     XR = XRR(40 + I) * DLTA
      YR=YRR(I) * DLTA
C     YR = YRR(40+I) * DLTA
      ZRL = ZR
      ZR = ZRR(I)
      IF (ZR - ZRL) 70,80,70
   70 CONTINUE
      CALL EXPZB
   80 CONTINUE
      CALL CONTR
      CALL POINT
          IF (IERR) 90,100,90
   90 CONTINUE
      WRITE (IPRTR,1001) YEAR,AMON,DAY,HOUR
      GO TO 160
```

```
  100 CONTINUE
      CAREA(I) = CONC
      CPOIN(I) = CONPS
      CNCT(I)= CONC+CONPS
C CONVERT CONCENTRATIONS FROM GRAM/SEC TO MICROGRAM/SEC
      CNCT(I) = 1.E6 * CNCT(I)
  140 CONTINUE
      CALL OUTPT
      GO TO 160
  150 CONTINUE
      WRITE(IPRTR,1003) WSPD,THTA
 1003 FORMAT (' WIND INPUT IS UNACCEPTABLE,WSPD=',F6.1
    1,',  THTA =',F7.3)
  160 CONTINUE
      CALL       INCRT
      IF(1.-STOP) 20,170,20
  170 CONTINUE
      REWIND 18
      CALL EXIT
      END
```

```
      SUBROUTINE OUTPT
      DIMENSION CNCT(50),CAREA(50),CPCIN(50),XRR(50),YRR(50)
     1,ZRR(50),OBSO2(50)
      DIMENSION DISTX(1000),XDCAY(2000),SSIGZ(1000),EXPOZ(2000)
     1,HA(5),UHA(5),QXY(5),Q(4000)
      DIMENSION XP (100),YP (100),ZP (100),QP(100)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/OUTPUT/YEAR,AMON,DAY,HOUR  ,NRECP,CNCT,CAREA,CPCIN
     1,XRR,YRR,ZRR,OBSO2,IDOW,NR1,TEMP,SIGA,RIB,PCPN,WGLD,STAPR
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,NH,HA
      1,UHA,QXY,Q,CONC,NH1
      COMMON/WNDSP/WSPD,WHGT,PWIND
      COMMON/POINTS/NPS   ,XP ,YP ,ZP ,QP,CONPS,NPSS
      DATA IWOF/18/
CCOMPUTE RECORD INDEX NUMBER
      Y     = HOUR + 100 * DAY + 1.E4 * AMON
C WRITE DATA INTO FILE
      WRITE(IWOF      )Y,YEAR,AMON ,DAY,IDOW,HOUR,NRECP
     1,(OBSO2(N),N=1,NRECP),(CNCT(N),N=1,NRECP)
     2,WSPD,WHGT,PWIND,THTA,INDEX,TEMP,CIGMX,SIGA,RIB,PCPN,WGLD,STAPR
C    1, (OBSO2(N),N=41,50),(CNCT(N),N=1,NRECP)
      WRITE(IPRTR,107) Y,IWOF
  107 FORMAT(' OUTPUT RECORD INDEX =',F10.0,', WRITTEN ON UNIT',I6)
      RETURN
      END
      SUBROUTINE DAFIL
C ROUTINE TO TRANSFER MODEL INPUTS FROM DISK AND TAPE TO CORE,
C ST.LOUIS DATA
      DIMENSION CNCT(50),CAREA(50),CPOIN(50),XRR(50),YRR(50)
     1,ZRR(50),OBSO2(50)
      DIMENSION DISTX(1000),XDCAY(2000),SSIGZ(1000),EXPOZ(2000)
     1,HA(5),UHA(5),QXY(5),Q(4000)
      DIMENSION XP (100),YP (100),ZP (100),QP(100)
      DIMENSION DUM1(100)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/OUTPUT/YEAR,AMON,DAY,HOUR ,NRECP,CNCT,CAREA,CPOIN
     1,XRR,YRR,ZRR,OBSO2,IDOW,NR1,TEMP,SIGA,RIB,PCPN,WGLD,STAPR
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,NH,HA
      1,UHA,QXY,Q,CONC,NH1
      COMMON/WNDSP/WSPD,WHGT,PWIND
      COMMON/POINTS/NPS  ,XP ,YP ,ZP ,QP,CONPS,NPSS
      DATA NRECS/0/
CCOMPUTE RECORD INDEX NUMBER
      YMDH = HOUR + 100 * DAY
      IF (AMON  - 12) 1,3,2
    1 CONTINUE
      YMDH = YMDH + AMON  * 10000
    3 CONTINUE
C COMPUTE RECORD NUMBER, EXIT IF REQUESTED DATA IS NOT IN FILE
      IF (YEAR - 64) 2,4,18
    2 CONTINUE
      YMDH = HOUR + 100 * DAY + 10000 * AMON  + 1000000.* YEAR
      WRITE (IPRTR,100) YMDH
  100 FORMAT (' YMDH =',F9.0,', DATA PERIOD REQUESTED IS NOT'
     1,' IN FILE')
      CALL EXIT
C CHECK REQUEST AGAINST DECEMBER 1964 DATES 01/1500 TO 31/2400
    4 CONTINUE
      NREC = -14
      IF (AMON  - 12) 2,6,2
    6 CONTINUE
      IF (DAY - 1) 2,8,10
    8 CONTINUE
      IF (HOUR - 15) 2,10,10
   10 CONTINUE
      IF (DAY - 31) 12,12,2
   12 CONTINUE
      IF (HOUR) 2,2,14
   14 CONTINUE
      IF (HOUR - 24) 16,16,2
   16 CONTINUE
      NREC = NREC + 24 * (DAY - 1) + HOUR
      GO TO 30
   18 CONTINUE
      IF (YEAR - 65) 2,20,2
   20 CONTINUE
      IF (AMON  - 1) 2,22,24
C CHECK REQUEST AGAINST JANUARY 1965 DATES 01/0100 TO 31/2400
   22 CONTINUE
      NREC = 730
      IF (DAY) 2,2,23
   23 CONTINUE
      GO TO 10
   24 CONTINUE
      IF (AMON  - 2) 2,26,2
C CHECK REQUEST AGAINST FEBRUARY 1965 DATES 01/0100 TO 28/1400
   26 CONTINUE
      NREC = 1474
      IF (DAY) 2,2,27
   27 CONTINUE
      IF (DAY - 28) 12,28,2
   28 CONTINUE
      IF (HOUR - 14) 12,12,2
   30 CONTINUE
C READ DATA FROM DISK
      IF (NRECS) 2,31,32
   31 CONTINUE
      IF (NREC - 1556) 32,32,131
  131 CONTINUE
C WORKING ON SECOND TAPE REEL,SPACE UNIT 15 DOWN 1556 RECORDS
      NRECS = 1556
      DO 132 I=1,1556
      READ (15)
  132 CONTINUE
   32 CONTINUE
      IF (NREC - NRECS - 1) 36,33,38
   33 CONTINUE
      READ (    15     ) XNDX,YRFI,AMFI,DAFI,IDOW,HRFI,NR1,NRECP
C CHECK DISK INDEX NUMBER AGAINST COMPUTED RECORD INDEX NUMBER
      IF (XNDX - YMDH) 35,40,35
   35 CONTINUE
      WRITE(IPRTR,101) XNDX,YMDH
  101 FORMAT (' XNDX =',F7.0,', YMDH =',F7.0,', DISK AND'
     1,' COMPUTED RECORD INDEX NUMBERS DO NOT AGREE')
      CALL EXIT
   36 CONTINUE
      NRECC = NRECS - NREC + 1
      DO 37 I=1,NRECC
      BACKSPACE 15
      BACKSPACE 16
   37 CONTINUE
      GO TO 33
   38 CONTINUE
      NRECC = NREC - NRECS - 1
      DO 39 I=1,NRECC
      READ (    15     )
      READ (    16     )
   39 CONTINUE
      GO TO 33
   40 CONTINUE
      BACKSPACE 15
      READ (    15     ) XNDX,YRFI,AMFI,DAFI,IDOW,HRFI,NR1,NRECP,(XRR(I),
     1,I=1,NR1),(YRR(I),I=1,NR1),(ZRR(I),I=1,NR1),(OBSO2(I)
     2,I=1,NR1),(DUM1(I),I=1,NRECP),GX,GY,DLTA,NH,(HA(I),I=1,NH)
     3,NPS,(XP(I),I=1,NPS),(YP(I),I=1,NPS),(ZP(I),I=1,NPS)
     4,(QP(I),I=1,NPS),WSPD,WHGT,PWIND,THTA,INDEX,TEMP,CIGMX
     5,SIGA,RIB,PCPN,WGLD,STAPR
C READ DATA FROM TAPE
      NQ = GX * GY * NH
      READ (    16     ) XNDH,GX,GY,NH,(Q   (I),I=1,NQ)
C CHECK TAPE INDEX NUMBER AGAINST COMPUTED RECORD INDEX NUMBER
      IF (XNDH - YMDH) 55,60,55
   55 CONTINUE
      WRITE(IPRTR,102) XNDH,YMDH
  102 FORMAT (' XNDH =',F7.0,', YMDH =',F7.0,', TAPE AND'
     1,' COMPUTED RECORD INDEX NUMBERS DO NOT AGREE')
      CALL EXIT
   60 CONTINUE
      NRECS = NREC
      RETURN
      END
      SUBROUTINE CHIDA
C ROUTINE TO GET CHICAGO DATA MODEL INPUTS, ASSUMING DATA FILE STARTS OC
C ON JAN 1 67 AND ENDS 2300 JAN 31 67.
      DIMENSION CNCT(50),CAREA(50),CPCIN(50),XRR(50),YRR(50)
     1,ZRR(50),OBSO2(50)
      DIMENSION DISTX(1000),XDCAY(2000),SSIGZ(1000),EXPOZ(2000)
     1,HA(5),UHA(5),QXY(5),QSIJ(4000)
      DIMENSION XP (100),YP (100),ZP (100),QP(100)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/OUTPUT/YEAR,AMON,DAY,HOUR ,NRECP,CNCT,CAREA,CPCIN
     1,XRR,YRR,ZRR,OBSO2,IDOW,NR1,TEMP,SIGA,RIB,PCPN,WGLD,STAPR
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,NH,HA
     1,UHA,QXY,Q,CONC,NH1
      COMMON/WNDSP/WSPD,WHGT,PWIND
      COMMON/POINTS/NPS   ,XP  ,YP  ,ZP  ,QP,CONPS,NPSS
      DIMENSION             RES(600),COM(600),XIND(600)
      DIMENSION RES1(150),COM1(250)
      EQUIVALENCE (RES(468),RES1(1)),(COM(392),COM1(1))
      DATA   RES   /   48*0. ,5.70E5,6.80E5,18*0. ,1.22E6,9.60E5,4.E5,4*0.
     1,1.00E4,12*0. ,1.48E6,4.80E5,9.00E5,1.60E5,4.00E4,0.00E0,8.E4
     2,1.10E5,12*0. ,1.90E6,8.70E5,1.08E6,9.20E5,2*8.E4,3.00E4,12*0.
     3,1.20E5,3.28E6,1.17E6,1.50E6,1.05E6,4.40E5,1.90E5,7.00E4,12*0.
     4,7.40E5,1.50E6,6.80E5,4.00E5,3.80E5,3.40E5,5.50E5,1.00E5,1.E4,5.E4
     5,10*0. ,9.00E5,1.01E6,5.00E4,8.10E5,1.12E6,3.50E5,5.70E5,2.5E5
     6,1.00E5,11*0. ,7.40E5,3.30E5,1.10E5,6.40E5,7.40E5,3.10E5,3.6E5
     7,2.70E5,8.00E4,10*0. ,1.50E5,3.70E5,3.00E4,8.20E5,1.15E6,6.3E5
     8,3.90E5,6.70E5,2.40E5,12*0. ,1.30E5,1.60E5,4.90E5,5.40E5,8.5E5
     9,5.40E5,6.20E5,4.00E5,13*0. ,1.60E5,5.80E5,9.40E5,1.92E6,1.17E6
     X,5.70E5,2.30E5,11*0. ,1.10E5,1.00E4,8.00E4,1.40E5,4.90E5,3.16E6
     1,7.60E5,14*0. ,9.00E4,2*0.   ,4.00E4,1.10E5,1.10E5,12*0. ,1.9E5
     2,6.40E5,1.10E5,7.00E4,1.40E5,4.00E4,14*0. ,5.60E5,2.64E6,5.E4,2*0.
     3,2*5.E4,12*0. ,1.00E5,1.21E6,2.19E6,1.80E5,1.10E5,1.00E5,4.E4,1.E5
     4,9.00E4,11*0. ,1.80E5,1.85E6,1.46E6,7.50E5,7.90E5,2.30E5,8.4E5
     5,2.70E5,3.00E4,0.00E0,1.00E4,9*0.   ,1.01E6,2.68E6,1.02E6,1.88E6
     6,1.07E6,4.40E5,7.60E5,3.00E4,1.00E4,10*0. ,7.00E5,1.14E6,4.3E5
     7,1.22E6,1.04E6,5.40E5,4.20E5,7.00E4,2.00E4,11*0. ,5.90E5,4.9E5
     8,1.14E6,1.29E6,1.20E5,1.06E6,6.20E5,12*0. ,5.00E4,3.60E5,9.E4
     9,2.80E5,2.80E5,1.10E5,3.50E5,7.00E4,12*0.,3.E4,5.E4,2*0.,6.E4/
      DATA RES1/
     X 1.00E5,9.00E4,13*0. ,1.80E5,1.00E4,2*0.   ,1.80E2,2.00E5,1.E5,2.E5
     1,5.00E4,3.00E4,14*0. ,3.30E5,1.30E5,1.00E4,2*3.E4,16*0. ,1.2E5
     2,14*0. ,4.00E4,2.00E4,56*0./
      DATA   COM     /48*0.,9.70E5,1.41E6,1.50E5,5*0.   ,1.30E5,11*0.
     1,2.46E6,1.51E6,5.50E5,3*0.   ,5.00E4,7.00E4,8.00E4,11*0. ,2.29E6
     2,9.30E5,6.10E5,4.10E5,3.20E5,1.10E5,1.00E5,2.00E5,1.70E5,11*0.
     3,2.88E6,1.02E6,9.10E5,8.10E5,2.10E5,1.90E5,1.30E5,7.00E4,1.4E5
     4,1.00E4,9*0.   ,6.70E5,3.90E6,1.66E6,7.40E5,1.13E6,7.70E5,3.15E6
     5,1.00E5,2*0.   ,6.00E4,9*0.   ,2.06E6,1.80E6,6.40E5,4.70E5,5.5E5
     6,4.70E5,3.30E5,2.70E5,1.10E5,5.00E4,2.00E4,9*0.   ,2.33E6,1.15E6
     7,1.13E6,6.30E5,1.02E6,7.20E5,3.60E5,2.30E5,2.90E5,11*0. ,2.12E6
     8,1.10E6,6.20E5,9.60E5,7.20E5,9.50E5,4.00E5,4.20E5,5.20E5,10*0.
     9,2.20E6,2.22E6,1.16E6,7.40E5,5.80E5,5.00E5,8.70E5,4.50E5,2.4E5
     X,11*0. ,4.40E6,2.86E6,1.81E6,9.80E5,1.40E6,9.70E5,1.27E6,1.44E6
     1,1.21E6,11*0. ,2.84E6,3.15E6,2.94E6,2.24E6,1.08E6,1.26E6,1.27E6
     2,1.13E6,9.20E5,11*0. ,2.03E6,1.02E6,1.45E6,5.60E5,9.70E5,8.6E5
     3,6.10E5,13*0. ,1.19E6,1.47E6,5.50E5,5.30E5,9.40E5,3.60E5,5.8E5
     4,12*0. ,1.72E6,6.60E5,1.92E6,1.84E6,6.60E5,6.60E5,4.20E5,1.9E5
     5,12*0. ,1.79E6,2.80E6,6.30E5,1.27E5,9.30E5,2.50E5,5.60E5,6.1E5
     6,1.20E5,10*0. ,9.40E5,2.39E6,2.50E6,4.10E5,1.69E6,6.00E5,6.6E5
     7,6.70E5,2.00E5,1.70E5,1.20E5,3.00E4,8*0.   ,2.40E5,2.48E6,1.93E6
     8,4.40E5,3.40E5,3.80E5,1.30E5,1.30E5,2.20E5,2.10E5,5.00E4,2.1E5
     9,7*0.   ,5.00E4,1.60E6,1.86E6,6.90E5,8.10E5,5.10E5,2.80E5,3.1E5/
      DATA COM1/
     X 9.00E4,8.00E4,1.40E5,9.50E5,4.00E4,7*0.   ,1.72E6,1.39E6,7.5E5
     1,1.70E5,6.00E5,7.70E5,2.60E5,2.10E5,2.00E5,5.50E5,9*0.   ,1.E4
     2,1.60E5,8.50E5,6.20E5,5.60E5,4.10E5,3.70E5,5.80E5,6.00E4,1.2E5
     3,1.1E5,9*0.,9.E4,4.6E5,1.1E5,2.60E5,9.00E4,8.00E4,1.40E5,1.1E5
     4,12*0. ,1.10E5,1.70E5,5.00E4,3.60E5,2.00E5,3.00E4,1.20E5,1.4E5
     5,7.00E4,4.70E5,10*0. ,1.70E5,1.82E6,0.00E0,2.50E5,2.50E5,1.3E5
     6,1.90E5,2.20E5,8.00E4,6.00E4,10*0. ,2.60E5,0.00E0,1.00E4,0.,6.5E5
     7,1.50E5,1.30E5,2.80E5,1.10E5,5.00E4,3.40E5,2*0.  ,1.00E5,3*0.,7.E4
     8,8.00E4,3.30E5,13*0. ,2.00E4,3.00E4,4.00E4,2.90E5,2.00E4,0.,3.E4
     9,13*0. ,2.00E4,2.60E5,0.00E0,1.00E4,4.40E5,33*0./
      DATA   XIND   /50*0. ,1.00E4,3*0.  ,1.00E4,13*0. ,8.00E4,2*1.E4
     1,21*0. ,5.00E4,2.00E4,0.00E4,1.00E4,12*0. ,1.00E4,2*3.E4,1.E4,2.E4
     2,5.00E4,1.00E4,13*0. ,3.00E4,7.00E4,4.00E4,2*2.E4,1.00E4,14*0.
     3,2*5.E4,7.00E4,5.40E5,5.00E4,1.00E4,13*0. ,1.00E4,4.20E5,2.4E6
     4,1.20E5,2.00E4,6.90E5,2*0.  ,6.00E4,11*0. ,2.40E5,7.20E6,8.8E5
     5,2.10E5,4.00E4,8.20E5,1.02E6,4.00E4,2.40E5,11*0. ,5.00E5,8.2E6
     6,2*7.E4,5.50E5,9.60E5,9.00E4,12*0. ,2.70E5,1.06E7,8.20E5,2.3E5
     7,8.10E5,8.00E4,5.00E5,7.00E4,1.00E4,11*0. ,6.00E5,2.20E5,1.2E5
     8,1.70E5,1.60E5,1.00E4,6.90E5,7.90E5,8.20E5,11*0. ,1.10E5,2.E4,2.E5
     9,1.70E5,6.10E5,4.00E4,9.10E5,13*0. ,2.30E5,1.75E6,2.22E6,2.1E5
     X,2.90E5,4.00E4,6.30E5,14*0. ,2.00E4,6.80E5,1.80E6,6.40E6,1.E5,3.E4
     1,13*0. ,7.00E5,1.50E6,9.46E6,1.58E6,2.80E6,5.80E5,6.40E5,12*0.
     2,1.00E4,0.00E0,6.00E4,4.00E4.5.80E5,3.10E5,9.00E4,2.00E4,12*0.
     3,2*1.E4,2*7.E4,1.00E4,8.80E5,4*0.  ,1.00E4,9*0.  ,1.00E4,2*2.E4,0.
     4,3.00E4,3*0.  ,3.00E4,10*0. ,1.00E4,4.00E4,1.00E4,2*5.E4,7.E4
     5,7.20E5,3.00E4,11*0. ,6.00E4,0.00E0,3.60E5,1.00E4,2.00E4,2*1.E4
     6,12*0. ,7.00E5,2.00E4,0.00E4,5.00E4,2*0.  ,1.00E4,13*0. ,6.E4,5.E4
     7,0.00E0,5.00E4,16*0. ,1.00E4,5.20E5,0.00E0,8.00E4,2*0.  ,1.5E5
     8,13*0. ,3.90E5,4.04E6,4*0.  ,2*1.E4,12*0. ,2.00E4,4.90E6,1.E4,0.
     9,3.00E4,0.00E0,2.24E6,15*0. ,5.00E4,18*0. ,6.90E5,36*0./
      DATA NRECS/0/
      IF (NRECS) 20,10,20
   10 CONTINUE
      REWIND 19
   20 CONTINUE
      YMDH = HOUR + 1.E2 * DAY + 1.E4 * AMON
C NREC SET BY COMPUTING NUMBER OF HOURS BY WHICH REQUESTED PERIOD EXCEED
C 0000 JAN 1 1967 PLUS 1
      NREC = (DAY - 1.) * 24. + HOUR + 1. + 1.
C ORIENT DATA FILE READER AT PROPER RECORD
C NRECS = RECORD NUMBER OF LAST RECORD READ
      NRECC = NREC - NRECS - 1
      IF (NRECC) 80,300,100
   80 CONTINUE
      DO 90 I=1,NRECC
      BACKSPACE 19
   90 CONTINUE
      GO TO 300
  100 CONTINUE
      DO 110 I=1,NRECC
      READ (     19    )
  110 CONTINUE
  300 CONTINUE
C READ DATA FROM DISK
      READ  (     19     ) XNDX,CY,CM,CD,IDOW,CH,NRECP,(OBS(I),I=1,NRECP)
     1,GX,GY,DLTA,NH,(HA(I),I=1,NH),NRPNT
     2,(ZP(I),I=1,NRPNT),(QP(I),I=1,NRPNT),WS,WH,P,WD,INDEX,TEMP,CIGMX
     3,SIGA,RIB,PCPN,WGLD,STAPR
C CHECK DATA INDEX NUMBER AGAINST COMPUTED INDEX NUMBER
      IF (XNDX - YMDH) 340,350,340
  340 CONTINUE
      WRITE (IPRTR,101) XNDX,YMDH
  101 FORMAT (' XNDX =',F7.0,', YMDH =',F7.0,', DISK AND COMPUTED RECORD
     1 INDEX NUMBERS DO NOT AGREE')
      REWIND 19
      CALL EXIT
  350 CONTINUE
      NR1 = NRECP
      NRECS = NREC
C CONVERT FT TO M IN HA ARRAY
      DO 355 I=1,NH
      HA(I) = 0.3048 * HA(I)
  355 CONTINUE
      IHOUR = HOUR
      IF (IHOUR) 360,360,370
  360 CONTINUE
      IHOUR = 24
  370 CONTINUE
      CALL DOWCH(IDOW,ID)
      NG = GX * GY
      DO 380 I=1,NG
      I1 = NG + 1 - I
      I2 = I1+ NG
      I3 = I2 + NG
      CALL ASHE(TEMP,ID  ,IHOUR,RES(I),COM(I),XIND(I),QSIJ(I1),QSIJ(I3)
     1,QSIJ(I2))
  380 CONTINUE
      RETURN
      END

      SUBROUTINE DOWCH(IDOW,ID)
C ROUTINE TO CLASSIFY DAYS OF WEEK
C           DAY            INPUT(IDOW)  OUTPUT(ID)
C            MON                1          2
C            TUE                2          2
C            WED                3          2
C            THU                4          2
C            FRI                5          2
C            SAT                6          3
C            SUN OR HOL   7 TO 17          1
      IF (IDOW - 6) 20,30,10
   10 CONTINUE
      ID = 1
      GO TO 40
   20 CONTINUE
      ID = 2
      GO TO 40
   30 CONTINUE
      ID = 3
   40 CONTINUE
      RETURN
      END

      SUBROUTINE PRAMB
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
C            NLI = MAXIMUM NUMBER OF LOG INCREMENTS IN INTEGRATION
C           XONE = CLOSEST SOURCE DISTANCE USED (METERS)
C            CONX= LOGARITHMIC INCREMENT FOR INTEGRATION VARIABLES
C          ISIGD = INDICATES OPTION FOR DEFINING DIFFUSION PARAMETERS
C                          1 = MCELROY-POOLER PARAMETERS USING TURNER STAB.
C                          2 = MCELROY-POOLER PARAMETERS USING RICHARDSON NO.
C                          3 = MCELROY-POOLER PARAMETERS USING BROOKHAVEN STAB
C                          4 = PASQUILL PARAMETERS USING TURNER STABILITY CAT.
C          DECAY = DECAY CONSTANT (PER SEC)
      ICARD = 5
      IPRTR = 6
      NLI = 20
      XONE = 50.
      XMAX = 5.5E4
      RN = 1. / (NLI - 1)
      CONX = (XMAX / XONE)**RN
      ISIGD = 4
      DECAY=0.
      RETURN
      END
      SUBROUTINE ASHE(TEMP,ID,IH,RES,COM,XIND,QR,QC,QI)
C ASHE CALCULATES HOURLY EMISSION RATE FOR AREA SOURCES
C INPUTS  TEMP - AVERAGE TEMPERATURE
C         ID   - DAY OF WEEK INDEX  ( 1 - 3 ,1=H,2=W,3=S)
C         IH   - HOUR OF DAY  ( 1 - 24 )
C         RES  - RESIDENTIAL EMISSION RATE  (YEARLY)
C         COM  - COMMERCIAL EMISSION RATE (YEARLY)
C         XIND - INDUSTRAIL EMISSION RATE (YEARLY)
      DIMENSION TFR(24,3),TFCI(24,3)
      DIMENSION TFR2(24)  ,TFCI2(24)
      EQUIVALENCE (TFR2(1),TFR(1,3)),(TFCI2(1),TFCI(1,3))
      DATA TFR/  8.11,  9.07,  9.12,  8.15,  6.64,  4.76,  1.83,  0.15,
     1          -5.60, -7.61, -8.72, -7.84, -5.55, -5.87, -4.09, -2.86,
     2           1.50, -1.43, -0.41, -0.61, -1.49, -0.60,  1.23,  4.78,
     3          11.11, 10.61,  9.69,  8.54,  7.08,  3.13, -2.15, -7.32,
     4          -7.61, -8.85, -8.44, -7.46, -6.73, -6.25, -5.11, -4.08,
     5          -3.17, -2.41, -0.77, -0.01,  2.56,  3.22,  5.33,  9.11/
      DATA TFR2/
     6          10.08, 11.97,  9.69,  8.43,  6.65,  4.24,  1.85, -0.73,
     7          -6.30, -8.01, -7.26, -9.34, -8.28, -8.07, -7.78, -6.14,
     8          -5.28, -3.82, -1.73, -0.86,  2.31,  3.85,  5.71,  8.74/
      DATA TFCI/16.87, 17.82, 18.43, 16.90, 15.15, 12.86,  9.47,  8.63,
     1           6.01,  4.82,  2.64,  1.38,  0.30,  0.55,  2.98,  4.49,
     2           6.25,  8.70,  9.92, 10.10, 10.47, 12.01, 12.23, 12.03,
     3          13.32, 13.23, 12.54, 10.43,  5.64, -1.75, -8.04,-11.69,
     4         -13.91,-12.94,-12.43,-12.53,-12.39,-11.19, -9.62, -7.88,
     5          -4.37,  0.56,  4.55,  6.62,  9.08, 10.41, 11.53, 13.19/
      DATA TFCI2/
     6          17.03, 18.19, 16.30, 14.55, 10.17,  3.19, -0.13, -4.13,
     7          -7.14, -6.74, -7.00, -6.78, -7.11, -7.01, -3.84, -1.84,
     8          -0.66,  2.60,  5.97,  7.92,  8.90, 11.47, 13.48, 15.86/
C CON1 = ANNUAL DEGREE DAYS * 24. = 6155. * 24.
      DATA CON1/147720./
C MULTIPLY BY CONCE TO CONVERT LBS/HR TO GRAMS/SEC
      DATA CONCE/0.1260/
      QRA= .9*RES
      QRC= .1*RES/8760.
C QRA = TEMPERATURE  DEPENDENT PORTION OF RESIDENTIAL AREA SOURCE EMISSI
C QRC = HOT WATER REQUIREMENT
      DDR = 65. - (TEMP + TFR(IH,ID))
      IF (DDR) 4,5,5
    4 DDR = 0.
    5 CONTINUE
      QR= QRC +QRA*DDR/CON1
C QR = ADJUSTED RESIDENTIAL SOURCE EMISSION RATE
      QCA= .9 *COM
      QCC= .1*COM/8760.
      DDC = 65. - (TEMP + TFCI(IH,ID))
      IF (DDC) 6,7,7
    6 DDC = 0.
    7 CONTINUE
      QC= QCC+ QCA*DDC/CON1
      QI=XIND/8760.
C QR,QI,QC ARE IN UNITS OF LBS/HR- CONVERT TO GRAMS/SEC
      QR=QR*CONCE
      QC=QC*CONCE
      QI=QI*CONCE
      RETURN
      END
      SUBROUTINE DISTB
C ROUTINE TO SET DISTANCE DEPENDENT ARRAYS.
      DIMENSION DISTX(1000),XDCAY(2000),SSIGZ(1000),EXPOZ(2000)
     1,HA(5),UHA(5),QXY(5),Q(4000)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,NH,HA
      1,UHA,QXY,Q,CONC,NHI
      COMMON/WNDSP/WSPD,WHGT,PWIND
      DATA ISTRT/0/
      IF (ISTRT) 30,10,30
   10 CONTINUE
      ISTRT = 1
C SET DISTX ARRAY
      DISTX(1) = XONE
      DO 20 I=2,NXLIM
      J = I - 1
      DISTX(I) = CONX* DISTX(J)
      IF (DISTX(I) - DISTX(J) - DLTA) 16,16,14
   14 CONTINUE
      DISTX(I) = DISTX(J) + DLTA
   16 CONTINUE
      IF (DISTX(I) - XMAX) 18,24,24
   18 CONTINUE
   20 CONTINUE
      NMISS = (XMAX - DISTX(NXLIM))/DLTA + 1.
      WRITE (IPRTR,1001) NMISS,XMAX,DISTX(NXLIM)
 1001 FORMAT(1XI8,' MORE LOCATIONS REQUESTED FOR DISTX ARRAY, XMAX =',
     1 E10.3,', DISTX(LAST)=',E10.3)
      CALL EXIT
   24 CONTINUE
      NLI = I
   30 CONTINUE
C SET ARRAYS WHICH DEPEND ON DISTANCE AND METEOROLOGICAL CONDITIONS ONLY
C GET AREA SOURCE WIND SPEEDS FOR EACH EMISSION HEIGHT
      DO 40 IH=1,NH
      UHA(IH) =WSPD* (HA(IH)/WHGT)**PWIND
   40 CONTINUE
C CHECK THAT DIMENSION LIMIT NXZLM IS NOT EXCEEDED
      NHLI=NH*NLI
      IF (NHLI-NXZLM) 26,26,25
   25 CONTINUE
      WRITE (IPRTR,1004)NXZLM,NHLI
 1004 FORMAT('  NH * NLI      EXCEEDS DIMENSION LIMIT OF',I6,',    NH,=',I
     16,',    NLI=',I6)
      CALL EXIT
   26 CONTINUE
C GET TRAVEL DISTANCE DECAY FACTORS
      IK = 0
      DO 60 I=1,NLI
      IDCAY = 0
      XI = DISTX(I)
      DO 50 IH=1,NH
      IK = IK + 1
      IF (DECAY) 42,42,44
   42 CONTINUE
      XDCAY(IK) = 1.
      GO TO 46
   44 CONTINUE
      XDCAY(IK) = EXP(-DECAY * XI / UHA(IH))
      IF (XDCAY(IK) - 1.E-6 ) 45,46,46
   45 CONTINUE
      IDCAY = IDCAY + 1
      IF (IDCAY - NH) 60,55,55
   55 CONTINUE
      NXI = I
      GO TO 62
   46 CONTINUE
   50 CONTINUE
   60 CONTINUE
      NXI = NLI
   62 CONTINUE
C GET SIGMAZ PARAMETERS
      DO 130 I=1,NXI
      XW = DISTX(I)
      CALL SIGZZ
      IF (IERR) 67,68,67
   67 CONTINUE
      RETURN
   68 CONTINUE
      SSIGZ(I) = SIGZ
      IF(SIGZ-CIGMX)70,140,140
   70 CONTINUE
  130 CONTINUE
      KUTEX = NXI
      GO TO 160
  140 CONTINUE
      KUTEX = I
      DO 150 J=1,NXI
      SSIGZ(J) = CIGMX
  150 CONTINUE
  160 CONTINUE
      RETURN
      END


      SUBROUTINE CONTR
C ROUTINE TO COMPUTE CONCENTRATION AT RECEPTOR XR,YR,ZR FROM AREA SOURCE
C GIVEN BY ARRAY Q WITH DIMENSIONS GX,GY,NH.
C THE COMPUTATION IS MADE BY INTEGRATING THE EFFECTS FROM EACH HGT. AND
C SUMMING.
      DIMENSION DISTX(1000),XDCAY(2000),SSIGZ(1000),EXPOZ(2000)
     1,HA(5),UHA(5),QXY(5),Q(4000)
      DIMENSION SXI(5),          TERMA(5)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,NH,HA
     1,UHA,QXY,Q,CONC,NH1
C CONST = 1/(2*SQRT(2*PI))
      DATA CONST/0.199471/
C NHLIM IS DIMENSION LIMIT FOR SXI AND   'TERMA ARRAYS.
      DATA NHLIM/5/
      YW = 0.
      IF (NH - NHLIM) 3,3,2
    2 CONTINUE
      WRITE(IPRTR,1000) NHLIM,NH
 1000 FORMAT (' NH EXCEEDS DIMENSION LIMIT OF',I6,', NH =',I6,',  NH SET
     1TO LIMIT')
      NH1= NHLIM
      GO TO 4
    3 CONTINUE
      NH1 = NH
    4 CONTINUE
      DO 10 IH=1,NH1
      SXI(IH) = 0
      TERMA(IH) = 0
   10 CONTINUE
      XWL = DISTX(1)
      DO 110 I=1,NX
      XW = DISTX(I)
      CALL SCORD
      CALL GCHEK
      IF (IND) 120,50,120
   50 CONTINUE
      CALL RATE
      IF (I - 1) 60,60,80
   60 CONTINUE
      DO 70 IH=1,NH1
      TERMA(IH) = QXY(IH) * EXPOZ(IH)
   70 CONTINUE
      GO TO 100
   80 CONTINUE
      DO 90 IH=1,NH1
      K = (I -1) * NH + IH
      TERMB = QXY(IH) * EXPOZ(K)
      SXI(IH) = SXI(IH) + (TERMA(IH) + TERMB) * (XW - XWL)
      TERMA(IH) = TERMB
   90 CONTINUE
  100 CONTINUE
      XWL = XW
  110 CONTINUE
      I1 = NX + 1
      IF (I1 - NLI) 115,115,140
  115 CONTINUE
      XW = DISTX(I1)
  120 CONTINUE
      DO 130 IH=1,NH1
      SXI(IH) = SXI(IH) + TERMA(IH) * (XW - XWL)
  130 CONTINUE
  140 CONTINUE
      CONC = 0
      DO 150 IH=1,NH1
      CONC = CONC + SXI(IH) / UHA(IH)
  150 CONTINUE
      CONC = CONST * CONC
      RETURN
      END



      SUBROUTINE RATE
C A SUBROUTINE TO INTERPOLATE EMISSION RATE OF A POINT INTERMEDIATE TO
C POINTS ON A STANDARD GRID SYSTEM
      DIMENSION DISTX(1000),XDCAY(2000),SSIGZ(1000),EXPOZ(2000)
     1,HA(5),UHA(5),QXY(5),Q(4000)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,NH,HA
     1,UHA,QXY,Q,CONC,NH1
C INITIALIZE INTEGER CONSTANTS
      IGRD = GX
      JGRD = GY
      NG = IGRD * JGRD
      X = XS/ DLTA
      IX = X
      Y = YS/ DLTA
      IY = Y
C CHECK IF POINT IS ON OUTSIDE FRINGE OF GRID, I.E. WITHIN 0.5 GRIDS OF
C EDGE.  IF POINT IS IN FRINGE CORNER, USE CORNER GRID VALUES.  OTHER
C POINTS, LINEARLY INTERPOLATE BETWEEN EDGE GRID POINTS.
      IF (X - IGRD) 10,1,1
    1 CONTINUE
      IF (Y - JGRD) 5,2,2
    2 CONTINUE
      K = 0
    3 CONTINUE
C USE CORNER VALUE.
      DO 4 I=1,NH1
      K = K + NG
      QXY(I) = Q(K)
    4 CONTINUE
      RETURN
    5 CONTINUE
      IF (IY) 6,6,7
    6 CONTINUE
      K = IGRD - NG
      GO TO 3
    7 CONTINUE
      K1 = IY * IGRD - NG
      K2 = K1 + IGRD
      DK = Y - IY
    8 CONTINUE
C USE LINEAR INTERPOLATION ON EDGE
      DO 9 I=1,NH1
      K1 = K1 + NG
      K2 = K2 + NG
      QXY(I) = Q(K1) + DK * (Q(K2) - Q(K1))
    9 CONTINUE
      RETURN
   10 CONTINUE
      IF (IX) 11,11,16
   11 CONTINUE
      IF (Y - JGRD) 13,12,12
   12 CONTINUE
      K = 1 - IGRD
      GO TO 3
   13 CONTINUE
      IF (IY) 14,14,15
   14 CONTINUE
      K = 1 - NG
      GO TO 3
   15 CONTINUE
      K2 = IY * IGRD + 1 - NG
      K1 = K2 - IGRD
      DK = Y - IY
      GO TO 8
   16 CONTINUE
      IF (Y -JGRD) 18,17,17
   17 CONTINUE
      K1 = IX - IGRD
      K2 = K1 + 1
      DK = X - IX
      GO TO 8
   18 CONTINUE
      IF (IY) 19,19,20
   19 CONTINUE
      K1 = IX - NG
      K2 = K1 + 1
      DK = X - IX
      GO TO 8
   20 CONTINUE
C DETERMINE WHICH TRIANGLE OF GRID POINTS WILL BE USED FOR INTERPOLATION
      BX = X - IX
      BY = Y - IY
      IF (BX - BY) 200,100,100
  100 CONTINUE
      K1 = IX + (IY - 1) * IGRD - NG
      DO 150 I=1,NH1
      K1 = K1 + NG
      K2 = K1+ 1
      K4 = K2 + IGRD
      QXY(I)=Q(K1)    + BX * ( Q(K2      )-Q(K1    ))+BY*(Q(K4)- Q(K2))
  150 CONTINUE
      RETURN
  200 CONTINUE
      K1 = IX + (IY - 1) * IGRD - NG
      DO 300 I=1,NH1
      K1 = K1 + NG
      K3 = K1 + IGRD
      K4 = K3 + 1
      QXY(I)=Q(K1)    + BY * (Q(K3      )-Q(K1    ))+BX*(Q(K4) - Q(K3))
  300 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE EXPZB
C ROUTINE TO COMPUTE VERTICAL DIFFUSION FACTOR INCLUDING EFFECTS OF
C    DECAY AND GROUND REFLECTIONS FOR EACH OF NH SOURCE HEIGHTS.
C BASIC EQUATION IS
C          EXPOZ = ( XDCAY / SIGZ )*(EXP(-0.5*((HA-ZR)/SIGZ)**2) +
C                                   EXP(-0.5*((HA+ZR)/SIGZ)**2))
      DIMENSION DISTX(1000),XDCAY(2000),SSIGZ(1000),EXPOZ(2000)
     1,HA(5),UHA(5),QXY(5),Q(4000)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,NH,HA
     1,UHA,QXY,Q,CONC,NH1
C  INPUTS
C                  ZR = RECEPTOR HEIGHT
C                  NH = NUMBER OF SOURCE HEIGHTS
C                  HA = ARRAY OF SOURCE HEIGHTS
C               CIGMX = MIXING CEILING
C               SSIGZ = VERTICAL DIFFUSION PARAMETER
C  OUTPUT
C               EXPOZ = VERTICAL DIFFUSION FACTOR
      K = 0
      DO 60 J=1,NXI
      G = 2. *CIGMX/SSIGZ(J)
      DO 50 I=1,NH
      F = (HA(I) - ZR) /SSIGZ(J)
      IF (F*F -  50.) 12,12,10
   10 CONTINUE
      E1 = 0
   11 CONTINUE
      E2 = 0
      GO TO 15
   12 CONTINUE
      E1 = EXP(-0.5 * F * F)
      F = (HA(I) + ZR) /SSIGZ(J)
      IF (F- 7.) 13,13,11
   13 CONTINUE
      E2 = EXP(-0.5 * F * F)
   15 CONTINUE
      K = K + 1
      EXPOZ(K) =((E1 + E2)      /SSIGZ(J)) * XDCAY(K)
   50 CONTINUE
   60 CONTINUE
      NX = NXI
      RETURN
      END
      SUBROUTINE INCRT
C THIS SUBROUTINE INCREMENTS THE TIME AT CONCENTRATIONS ARE CALC. BY THE
C DIFFUSION PROGRAM. IN ADDITION TO THIS IT GENERATES THE TIME INDEX
C WHICH IS USED TO GENERATE THE SOURCE MATRIX AND METEOROLOGICAL INPUTS
C CORRESPONDING TO THE TIME AT WHICH THE CONCENTRATION IS REQUIRED.
      DIMENSION YEARR(2),AMONN(2),DAYY(2),HOURR(2)
      COMMON/DATIME /DH,STOP,YEARR,AMONN,DAYY,HOURR,HOURL
      DIMENSION DIM(12)
C DIM IS AN ARRAY REPRESENTING THE NUMBER OF DAYS IN EACH MONTH
      DATA DIM/31.,28.,31.,30.,31.,30.,31.,31.,30.,31.,30.,31./
C THE ARRAYS YEARR, AMONN, DAYY, HOURR CONTAIN THE YEAR (TWO DIGITS),MO.
C DAY, AND HOUR OF THE FIRST AND LAST CALCULATION (INDEX=1 AND INDEX=2
C RESPECTIVELY)
C CHECK FOR LEAP YEAR
      TEST= YEARR(1) / 4.
      ITEST=TEST
      IF(TEST-ITEST) 200,100,200
  100 CONTINUE
C YEAR(1) IS A LEAP YEAR
      DIM(2)=29.
      GO TO 220
  200 CONTINUE
      DIM(2) = 28.
  220 CONTINUE
C INCREMENT HOUR
      HOURR(1) = HOURR(1) + DH
C CHECK TO SEE IF HOUR(1) IS IN THE SAME DAY
      IF(HOURR(1)-HOURL) 600,600,300
  300 CONTINUE
C HOUR(1) IS NOT IN THE SAME DAY
      HOURR(1) = HOURR(1) - 24.
      DAYY(1) = DAYY(1) + 1.
C CHECK TO SEE IF DAY(1) IS IN THE SAME MONTH
      MONTH=AMONN(1)
      IF (DAYY(1) - DIM(MONTH)) 600,600,400
  400 CONTINUE
C DAY(1) IS NOT IN THE SAME MONTH
      AMONN(1) = AMONN(1) + 1.
      DAYY(1) = DAYY(1) - DIM(MONTH)
C CHECK TO SEE IF MONTH(1) IS IN SAME YEAR
      IF(AMONN(1)-12.) 600,600,500
  500 CONTINUE
C MONTH(1) IS NOT IN THE SAME YEAR
      AMONN(1) = AMONN(1) - 12.
      YEARR(1) = YEARR(1) + 1.
  600 CONTINUE
C CHECK TO SEE IF THIS IS LAST INCREMENT
      IF (YEARR(1) - YEARR(2)) 1100,700,1000
  700 CONTINUE
C YEARS ARE THE SAME
      IF(AMONN(1)-AMONN(2)) 1100,800,1000
  800 CONTINUE
C MONTHS ARE THE SAME
      IF (DAYY(1) - DAYY(2)) 1100,900,1000
  900 CONTINUE
C DAYS ARE THE SAME
      IF (HOURR(1) - HOURR(2)) 1100,1100,1000
 1000 CONTINUE
C STOP INCREMENTING
      STOP=1.
      RETURN
 1100 CONTINUE
      STOP=0.
      RETURN
      END
```

Exhibit D-2

LISTING OF FORTRAN CODE COMPUTER PROGRAM AND SUBROUTINES USED FOR SENSITIVITY CALCULATIONS*

*Additional subroutines are listed in Exhibit D-3.

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C DIFFUS3 - SENSITIVITY ANALYSIS
      DIMENSION DTHTA(10)
      DATA DTHTA/-45.,-10.,-3.,0.,3.,10.,45./
      DIMENSION YEARR(2),AMONN(2),DAYY(2),HOURR(2)
      DIMENSION CNCT(50),CAREA(50),CPOIN(50),XRR(50),YRR(50),ZRR(50)
     1,OBSO2(50),OSET(12,54)
      DIMENSION DISTX(200,7),XDCAY(600,7),SSIGZ(200,7),EXPOZ(600,7)
     1,HA(5),UHA(5),QXY(5),Q(3600),QX(200,3,1,7),NQX(7,3)
      DIMENSION XP (100),YP (100),ZP (100),QP(100)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE,XMAX,CONX
     1,DECAY,INDEX,THTA,CIGMX,GX,GY, DLTA,IND,SIGY,SIGZ,XR,YR,ZR,XS,YS
     2,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/DATIME /DH,STOP,YEARR,AMONN,DAYY,HOURR
      COMMON/OUTPUT/YEAR,AMON,DAY,HOUR ,NRECP,CNCT,CAREA,CPOIN,XRR,YRR
     1,ZRR,OBSO2,IDOW,NR1,TEMP,SIGA,RIB,PCPN,WGLD,STAPR,OSET,INDO
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,   NH,HA,UHA
     1, QXY,Q    ,CONC,NH1,QX,NQX
      COMMON/WNDSP/WSPD,WHGT,PWIND
      COMMON/POINTS/NPS  ,XP ,YP ,ZP ,QP,CONPS,NPSS
C SET CONTROL PARAMETERS
      IERR = 0
      INDO = 0
      ICARD = 5
      IPRTR = 6
      NLI = 20
      XMAX = 5.5E4
      XONE = 1.
      RN = 1. / (NLI - 1)
      CONX = (XMAX / XONE)**RN
C GET BASE EMISSION FIELD, RECEPTOR LOCATIONS AND WIND DIRECTION
      CALL SENDA
      WRITE(IPRTR,901) ICARD,IPRTR,XONE,XMAX,CONX
  901 FORMAT(/' CONTROL PARAMETERS'/4X'ICARD',3X'IPRTR',8X'XONE',8X'XMAX
     1',8X'CONX'/1X2I8,3E12.3/)
      XYMIN = 0.5 * DLTA
      XSMAX = (GX + 0.5) * DLTA
      YSMAX = (GY + 0.5) * DLTA
C GET QX ARRAY
   20 CONTINUE
      THTA1 = THTA
      CALL GENQX
      IF (IERR) 150,30,150
   30 CONTINUE
      IO = 0
C CYCLE ON DIFFUSION PARAMETERS
      DO 148 I8=1,3
      GO TO (45,46,47),I8
   45 CONTINUE
      ISIGD = 4
      INDEX = 5
      GO TO 48
   46 CONTINUE
      ISIGD = 1
      INDEX = 4
      GO TO 48
   47 CONTINUE
      ISIGD = 2
      INDEX = 1
   48 CONTINUE
C CYCLE ON MIXING CEILING
      CIGMX = 20.
      DO 147 I7=1,2
      CIGMX = 5. * CIGMX
      ISTAR = 0
      CALL SIGZZ
      ISTAR = 1
      IF (IERR) 150,50,150
   50 CONTINUE
```

```
C CYCLE ON WIND PROFILE POWER
      PWIND = 0.075
      DO 146 I6=1,1
      PWIND = 2. * PWIND
C CYCLE ON WIND SPEED
      WSPD = 2. / 3.
      DO 145 I5=1,3
      WSPD = 3. * WSPD
      WRITE (IPRTR,900)
  900 FORMAT(//'1 INDO',2X'AREA CONC.',3X'PT. CONC.'
     A                  ,2X'TOT. CONC.',3X'ISIGD',3X'INDEX',3X'CIGMX',3X
     1'PWIND',4X'WSPD',3X'DECAY',3X'NH',4X'THTA',3X'NPS',2X'RECEPTOR'/)
C CYCLE ON DECAY CONSTANT
      DO 144 I4=1,1
      GO TO (51,52,53),I4
   51 CONTINUE
      DECAY = 0.
      GO TO 54
   52 CONTINUE
      DECAY = 0.0003851
      GO TO 54
   53 CONTINUE
      DECAY = 0.05
   54 CONTINUE
C CYCLE ON DISTRIBUTION OF EMISSION HEIGHTS
      DO 143 I3=1,1
      GO TO (55,56),I3
   55 CONTINUE
      NH = 1
      HA(1) = 30.
      GO TO 57
   56 CONTINUE
      NH = 3
      HA(1) = 15.
      HA(2) = 30.
      HA(3) = 45.
   57 CONTINUE
      CALL DISTC
      IF (IERR) 150,58,150
   58 CONTINUE
      CALL EXPZC
C CYCLE ON GRID SPACING
      DO 142 I2=1,7
      THTA = THTAI+ DTHTA(I2) * 3.14159 / 180.
      ISTAR = 0
      CALL SCORD
      CALL WCORD
      ISTAR = 1
C CYCLE ON NUMBER OF POINT SOURCES
      DO 141 I1=1,1
      GO TO (65,66,67),I1
   65 CONTINUE
      NPSS = 51
      GO TO 68
   66 CONTINUE
      NPSS = 19
      GO TO 68
   67 CONTINUE
      NPSS = 0
   68 CONTINUE
C CYCLE ON RECEPTOR LOCATION
      DO 140 I=1,3
      INDO = INDO + 1
      IO = IO + 1
      XR = XRR(I)
      YR = YRR(I)
      CALL CONTRS(I,I1,I2)
      CONPS = 0.
      IF (NPS) 100,100,85
   85 CONTINUE
      CALL POINT
      IF (IERR) 90,100,90
   90 CONTINUE
      WRITE(IPRTR,1002) INDO
 1002 FORMAT(/' ERROR RETURN FROM POISN, INDO =',I8/)
      GO TO 150
  100 CONTINUE
      OSET(1 , IO)    = CONC * 1.E6
      OSET( 2, IO   ) = CONPS * 1.E6
      OSET( 3, IO   ) =(CONC + CONPS) * 1.E6
      OSET( 4, IO   ) = NPS
      OSET( 5, IO   ) = THTA
      OSET( 6, IO   ) = NH
      OSET( 7, IO   ) = DECAY
      OSET( 8, IO   ) = WSPD
      OSET( 9, IO   ) = PWIND
      OSET(10, IO   ) = CIGMX
      OSET(11, IO   ) = ISIGD
      OSET(12, IO   ) = XRR(I)
      WRITE(IPRTR,902) INDO,(OSET(N,IO),N=1,3),ISIGD,INDEX,CIGMX
     1,PWIND,WSPD,DECAY,NH,THTA,NPS,XRR(I)
  902 FORMAT(1X15,3E12.3,2I8,F8.0,F8.3,F8.1,F8.3,I5,F8.3,I6,F9.0)
  140 CONTINUE
  141 CONTINUE
  142 CONTINUE
  143 CONTINUE
  144 CONTINUE
      CALL OUTSE
      IO = 0
  145 CONTINUE
  146 CONTINUE
  147 CONTINUE
  148 CONTINUE
  149 CONTINUE
      THTA = 0.35
      GO TO 20
  150 CONTINUE
      END FILE 12
      CALL EXIT
      END


      SUBROUTINE GENQX
      DIMENSION QA(3),QB(3),QC(3)
      DIMENSION QR(4,4)
      DIMENSION DTHTA(10)
      DATA DTHTA/-45.,-10.,-3.,0.,3.,10.,45./
      DIMENSION CNCT(50),CAREA(50),CPCIN(50),XRR(50),YRR(50),ZRR(50)
     1,OBSO2(50),OSET(12,54)
      DIMENSION DISTX(200,7),XDCAY(600,7),SSIGZ(200,7),EXPOZ(600,7)
     1,HA(5),UHA(5),QXY(5),Q(3600),QX(200,3,1,7),NQX(7,3)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE,XMAX,CON
     1,DECAY,INDEX,THTA,CIGMX,GX,GY, DLTA,IND,SIGY,SIGZ,XR,YR,ZR,XS,YS
     2,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/OUTPUT/YEAR,AMON,DAY,HOUR ,NRECP,CNCT,CAREA,CPCIN,XRR,YRR
     1,ZRR,OBSO2,IDOW,NR1,TEMP,SIGA,RIB,PCPN,WGLD,STAPR,OSET,INDO
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,    NH,HA,UHA
     1, QXY,Q    ,CONC,NH1,QX,NQX
      NXLIM = 200
      YW = 0.
      THTA1 = THTA
      DO 10 J=1,3
      DO 10 I=1,7
      NQX(I,J) = 0
   10 CONTINUE
      READ (ICARD,1000) IR1
 1000 FORMAT (I10)
      WRITE(IPRTR,1001) IR1
 1001 FORMAT(/' INITIAL RANDOM NO. INTEGER =',I10)
      IRS = IR1
      GX = 120.
      GY = 160.
      DLTA = 381.
      DO 200 IB=1,7
      IR1 = IRS
      THTA = THTA1+ DTHTA(IB) * 3.14159 / 180.
      ISTAR = 0
      CALL SCORD
      CALL WCORD
      ISTAR = 1
C SET DISTX ARRAY
      DISTX(1,IB) = XONE
      DO 20 I=2,NXLIM
      J = I - 1
      DISTX(I,IB) = CONX * DISTX(J,IB)
      IF (DISTX(I,IB) - DISTX(J,IB) - DLTA) 16,16,14
   14 CONTINUE
      DISTX(I,IB) = DISTX(J,IB) + DLTA
   16 CONTINUE
      IF ( DISTX(I,IB) - XMAX) 18,24,24
   18 CONTINUE
   20 CONTINUE
      NMISS = (XMAX - DISTX(NXLIM,IB)) / DLTA + 1.
      WRITE (IPRTR,1002) NMISS,XMAX,DISTX(NXLIM,IB)
 1002 FORMAT(1X18,' MORE LOCATIONS REQUESTED FOR DISTX ARRAY, XMAX =',
     1 E10.3,', DISTX(LAST)=',E10.3)
      IERR = 1
      RETURN
   24 CONTINUE
      NLI = I
      DO 300 IC=1,3
      XR = XRR(IC)
      YR = YRR(IC)
      KLAST = 0
      DO 100 J=1,NLI
      XW = DISTX(J,IB)
      CALL SCORD
      CALL GCHEKS
      IF (IND) 110,40,110
   40 CONTINUE
   50 CONTINUE
      IX1 = XS / 1524. + 0.5
      IY1 = YS / 1524. + 0.5
      K = (IY1 - 1) * 30 + IX1
      IF (K - KLAST) 51,52,51
   51 CONTINUE
C GENERATE SUB-GRID FOR BLOCK K EMISSIONS
      KLAST = K
      QM = Q(K)
      CALL QAREA(IR1,QM,QR)
      IF ( IERR) 360,52,360
   52 CONTINUE
      IX = XS / DLTA - 1.
      IY = YS / DLTA - 1.
      IX2 = IX - 4 * (IX1 - 1)
      IY2 = IY - 4 * (IY1 - 1)
      QX(J,IC,1,IB) = QR(IX2,IY2)
  100 CONTINUE
      NQX(IB,IC) = NLI
      GO TO 300
  110 CONTINUE
      NQX(IB,IC) = J - 1
```

```
300 CONTINUE
200 CONTINUE
    IF (NQX(1,1) - NQX(1,2)) 340,310,310
310 CONTINUE
    IF (NQX(1,1) - NQX(1,3)) 330,320,320
320 CONTINUE
    ICX = 1
    GO TO 360
330 CONTINUE
    ICX = 3
    GO TO 360
340 CONTINUE
    IF (NQX(1,2) - NQX(1,3)) 330,350,350
350 CONTINUE
    ICX = 2
360 CONTINUE
    RETURN
    END


    SUBROUTINE SENDA
    DIMENSION ICP(100),XPP(100),YPP(100),ZPP(100)
    DIMENSION CNCT(50),CAREA(50),CPCIN(50),XRR(50),YRR(50),ZRR(50)
   1,OBSO2(50),OSET(12,54)
    DIMENSION DISTX(200,7),XDCAY(600,7),SSIGZ(200,7),EXPOZ(600,7)
   1,HA(5),UHA(5),QXY(5),Q(3600),QX(200,3,1,7),NQX(7,3)
    DIMENSION XP (100),YP (100),ZP (100),QP(100)
    COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE,XMAX,CCN
   1,DECAY,INDEX,THTA,CIGMX,GX,GY, DLTA,IND,SIGY,SIGZ,XR,YR,ZR,XS,YS
   2,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
    COMMON/OUTPUT/YEAR,AMON,DAY.HOUR ,NRECP,CNCT,CAREA,CPCIN,XRR,YRR
   1,ZRR,OBSO2,IDOW,NR1,TEMP,SIGA,RIB,PCPN,WGLD,STAPR,OSET,INDC
    COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,    NH,HA,UHA
   1, QXY,Q    ,CONC,NH1,QX,NQX
    COMMON/WNDSP/WSPD,WHGT,PWIND
    COMMON/POINTS/NPS   ,XP  ,YP  ,ZP  ,QP,CONPS,NPSS
    READ (10) YMDH, DLTA,GX,GY,WHGT,THTA,NH,NPS,(XPP(N),YPP(N),ZPP(N)
   1,QP(N),N=1,NPS)
    NG = GX * GY
    DO 50 I=1,NH
    N1 = (I -1) * NG
    READ (10) (Q(N+N1),N=1,NG)
 50 CONTINUE
    XRR(2) = 16.5 * DLTA
    YRR(2) = 20.5 * DLTA
    XRR(1) = XRR(2) +  9. * DLTA *  TAN(THTA)
    YRR(1) = 29.5 * DLTA
    XRR(3) = XRR(2) - 18. * DLTA *  TAN(THTA)
    YRR(3) =  2.5 * DLTA
    ZR = 0.
    DO 55 I=1,NPS
    ICP(I) = I
 55 CONTINUE
    CALL SORT1(ICP)
    DO 60 I=1,NPS
    J = ICP(I)
    XP(I) = XPP(J)
    YP(I) = YPP(J)
    ZP(I) = ZPP(J)
 60 CONTINUE
    AREA = DLTA * DLTA
    DO 70 I=1,NG
    Q(I) = Q(I) + Q(I+NG) + Q(I+2*NG)
    Q(I) = Q(I) / AREA
 70 CONTINUE
    RETURN
    END
```

```
      SUBROUTINE SORT1 (ICP)
      DIMENSION ICP(1)
      DIMENSION CP(100)
      DIMENSION XP (100),YP (100),ZP (100),QP(100)
      COMMON/POINTS/NPS  ,XP ,YP ,ZP ,QP,CONPS,NPSS
      EQUIVALENCE (CP(1),QP(1))
      ITEMS = NPS
      NP = ITEMS
    1 NP = NP/2
      IF(NP) 7,7,2
    2 K = ITEMS - NP
      J = 1
    3 I = J
      M = I + NP
    4 IF (CP(I) - CP(M)) 6,6,5
    5 SAVE = CP(I)
      CP(I) = CP(M)
      CP(M) = SAVE
      ISAVE = ICP(I)
      ICP(I)= ICP(M)
      ICP(M)= ISAVE
      M = I
      I = I - NP
      IF (I - 1) 6,4,4
    6 J = J + 1
      IF (J - K) 3,3,1
    7 RETURN
      END
```

```
      SUBROUTINE QAREA(IR1,QM,QR)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE,XMAX,CCN
     1,DECAY,INDEX,THTA,CIGMX,GX,GY, DLTA,IND,SIGY,SIGZ,XR,YR,ZR,XS,YS
     2,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      DIMENSION QR(4,4)
      DO 40 J=1,4
      DO 30 I=1,4
      CALL RANDU(IR1,IR2,RFL)
      CALL NDTRI(RFL,QN,QD,IER)
      IF (IER) 10,20,10
   10 CONTINUE
      WRITE(IPRTR,1000) RFL,IR1,IR2
 1000 FORMAT(/' RANDOM NO. ERROR, RFL =',F10.5,' ,IR1 =',I10,', IR2 ='
     1,I10/)
      IERR = IER
      RETURN
   20 CONTINUE
      IR1 = IR2
      IF (QN + 2.) 25,25,26
   25 CONTINUE
      QR(I,J) = 0.
      GO TO 30
   26 CONTINUE
C USE STD. DEV. = 0.5 * MEAN
      QR(I,J)=(QN * 0.5 + 1.) * QM
   30 CONTINUE
   40 CONTINUE
      RETURN
      END
```

```
C        SUBROUTINE NDTRI
C           COMPUTES X = P**(-1)(Y), THE ARGUMENT X SUCH THAT Y=P(X) =
C           THE PROBABILITY THAT THE RANDOM VARIABLE U, DISTRIBUTED
C           NORMALLY(0,1), IS LESS THAN OR EQUAL TO X. F(X), THE
C           ORDINATE OF THE NORMAL DENSITY, AT X, IS ALSO COMPUTED.
C        DESCRIPTION OF PARAMETERS
C           P - INPUT PROBABILITY.
C           X - OUTPUT ARGUMENT SUCH THAT P = Y = THE PROBABILITY THAT
C                  U, THE RANDOM VARIABLE, IS LESS THAN OR EQUAL TO X.
C           D - OUTPUT DENSITY, F(X).
C           IER - OUTPUT ERROR CODE
C                 =-1 IF P IS NOT IN THE INTERVAL (0,1), INCLUSIVE.
C                 =0 IF THERE IS NO ERROR. SEE REMARKS, BELOW.
C        REMARKS
C           MAXIMUM ERROR IS 0.00045.
C           IF P = 0, X IS SET TO -(10)**74. D IS SET TO 0.
C           IF P = 1, X IS SET TO  (10)**74. D IS SET TO 0.
C        METHOD
C           BASED ON APPROXIMATIONS IN C. HASTINGS, APPROXIMATIONS FOR
C           DIGITAL COMPUTERS, PRINCETON UNIV. PRESS, PRINCETON, N.J.,
C           1955. SEE EQUATION 26.2.23, HANDBOOK OF MATHEMATICAL
C           FUNCTIONS, ABRAMOWITZ AND STEGUN,DOVER PUBLICATIONS, INC.,
C           NEW YORK.
      SUBROUTINE NDTRI(P,X,D,IE)
      IE=0
      IF(P)1,4,2
    1 IE=-1
      GO TO 12
    2 IF(P-1.0)7,6,1
    4 X=-.999999E+38
    5 D=0.0
      GO TO 12
    6 X=.999999E+38
      GO TO 5
    7 D=P
      IF(D-0.5)9,9,8
    8 D=1.0-D
    9 T2=ALOG(1.0/(D*D))
      T=SQRT(T2)
      X=T-(2.515517+0.802853*T+0.010328*T2)/(1.0+1.432788*T+0.189269*T2
     1  +0.001308*T*T2)
      IF(P-0.5)10,10,11
   10 X=-X
   11 D=0.3989423*EXP(-X*X/2.0)
   12 RETURN
      END
```

```
      SUBROUTINE RANDU(IX,IY,YFL)
      IY=IX*899
      IF(IY)5,6,6
    5 IY=IY+2147483647+1
    6 YFL=IY
      YFL=YFL/2147483647.
      RETURN
      END
      SUBROUTINE RATEA(J,IB,IC,X,Y)
C A SUBROUTINE TO INTERPOLATE EMISSION RATE OF A POINT INTERMEDIATE TO
C POINTS ON A STANDARD GRID SYSTEM
      DIMENSION QA(3),QB(3),QC(3)
      DIMENSION DISTX(200,3),XDCAY(600,3),SSIGZ(200,3),EXPOZ(600,3)
     1,HA(5),UHA(5),QXY(5),Q(3600),QX(200,3,3,3),NQX(3,3)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE,XMAX,CONX
     1,DECAY,INDEX,THTA,CIGMX,GX,GY, DLTA,IND,SIGY,SIGZ,XR,YR,ZR,XS,YS
     2,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,    NH,HA,UHA
     1, QXY,Q    ,CONC,NH1,QX,NQX
C INITIALIZE INTEGER CONSTANTS
      IGRD = GX + 0.5
      JGRD = GY
      NG = IGRD * JGRD
      IX = X
      IY = Y
C CHECK IF POINT IS ON OUTSIDE FRINGE OF GRID, I.E. WITHIN 0.5 GRIDS OF
C EDGE.  IF POINT IS IN FRINGE CORNER, USE CORNER GRID VALUES.  OTHER
C POINTS, LINEARLY INTERPOLATE BETWEEN EDGE GRID POINTS.
      IF (X - IGRD) 10,1,1
    1 CONTINUE
      IF (Y - JGRD) 5,2,2
    2 CONTINUE
      K = NG
    3 CONTINUE
C USE CORNER VALUE.
      GO TO (60,31,32),IB
   31 CONTINUE
      QA(1) = Q(K)
      IX1= X + 0.5
      X1 = IX1* DLTA
      IY1= Y + 0.5
      Y1 = IY1* DLTA
      GO TO 33
   32 CONTINUE
      IX1= X + 0.5
      IY1= Y + 0.5
      CALL QCOMB(IX1,IY1,QD)
      QA(1) = QD
      X1 = (IX1- 0.375) * DLTA
      Y1 = (IY1- 0.375) * DLTA
   33 CONTINUE
      QA(2) = QA(1)
      QA(3) = QA(1)
      IQI = 1
      CALL ADDPO(IQI,X1,Y1,QA,QB,QC)
      DO 35 I=1,3
      QX(J,IC,I,IB) = QA(I)
   35 CONTINUE
      GO TO 57
    5 CONTINUE
      IF (IY) 6,6,7
    6 CONTINUE
      K = IGRD
      GO TO 3
    7 CONTINUE
      K1 = IY * IGRD
      K2 = K1 + IGRD
      D1 = Y - IY
      IQI = 3
    8 CONTINUE
C USE LINEAR INTERPOLATION ON EDGE
      GO TO (60,41,42),IB
   41 CONTINUE
      QA(1) = Q(K1)
      QB(1) = Q(K2)
      IF (IQI - 3) 47,48,48
   47 CONTINUE
      X1 = IX * DLTA
      IY1 = Y + 0.5
      Y1 = IY1 * DLTA
      GO TO 45
   48 CONTINUE
      IX1 = X + 0.5
      X1 = IX1 * DLTA
      Y1 = IY * DLTA
      GO TO 45
   42 CONTINUE
      IF (IQI - 3) 43,44,44
   43 CONTINUE
      IY1 = Y + 0.5
      Y1 = IY1 * DLTA
      X1 = IX * DLTA
      CALL QCOMB(IX ,IY1,QD)
      QA(1) = QD
      IX1 = IX + 1
      CALL QCOMB(IX1,IY1,QD)
      QB(1) = QD
      GO TO 45
   44 CONTINUE
      IX1 = X + 0.5
      X1 = IX1 * DLTA
      Y1 = IY * DLTA
      CALL QCOMB(IX1,IY,QD)
      QA(1) = QD
      IY1 = IY + 1
      CALL QCOMB(IX1,IY1,QD)
      QB(1) = QD
   45 CONTINUE
      QA(2) = QA(1)
      QA(3) = QA(1)
      QB(2) = QB(1)
      QB(3) = QB(1)
      CALL ADDPU(IQI,X1,Y1,QA,QB,CC)
      DO 46 I=1,3
      QX(J,IC,I,IB) = QA(I) + D1*(QB(I) * QA(I))
   46 CONTINUE
      GO TO 57
   10 CONTINUE
      IF (IX) 11,11,16
   11 CONTINUE
      IF (Y - JGRD) 13,12,12
   12 CONTINUE
      K = 1 - IGRD + NG
      GO TO 3
   13 CONTINUE
      IF (IY) 14,14,15
   14 CONTINUE
      K = 1
      GO TO 3
   15 CONTINUE
      K2 = IY * IGRD + 1
      K1 = K2 - IGRD
      D1 = Y - IY
      IQI = 3
      GO TO 8
   16 CONTINUE
      IF (Y -JGRD) 18,17,17
   17 CONTINUE
      K1 = IX - IGRD + NG
      K2 = K1 + 1
      D1 = X - IX
      IQI = 2
      GO TO 8
   18 CONTINUE
      IF (IY) 19,19,20
   19 CONTINUE
      K1 = IX
      K2 = K1 + 1
      D1 = X - IX
      IQI = 2
      GO TO 8
   20 CONTINUE
C DETERMINE WHICH TRIANGLE OF GRID POINTS WILL BE USED FOR INTERPOLATIO
      D1 = X - IX
      D2 = Y - IY
      K1 = IX + (IY - 1) * IGRD
      IF (D1 - D2) 200,100,100
  100 CONTINUE
      K2 = K1 + 1
      K3 = K2 + IGRD
      IQI = 4
   50 CONTINUE
      GO TO (60,52,53),IB
   52 CONTINUE
      QA(1) = Q(K1)
      QB(1) = Q(K2)
      QC(1) = Q(K3)
      X1 = IX * DLTA
      Y1 = IY * DLTA
      GO TO 56
   53 CONTINUE
      CALL QCOMB(IX,IY,QD)
      QA(1) = QD
      IX1 = IX + 1
      IY1 = IY + 1
      CALL QCOMB(IX1,IY1,QD)
      QC(1) = QD
      X1 = (IX - 0.375) * DLTA
      Y1 = (IY - 0.375) * DLTA
      IF (IQI - 4) 54,54,55
   54 CONTINUE
      CALL QCOMB(IX1,IY,QD)
      QB(1) = QD
      GO TO 56
   55 CONTINUE
      CALL QCOMB(IX,IY1,QD)
      QB(1) = QD
   56 CONTINUE
      QA(2) = QA(1)
      QA(3) = QA(1)
      QB(2) = QB(1)
      QB(3) = QB(1)
      QC(2) = QC(1)
      QC(3) = QC(1)
      CALL ADDPO(IQI,X1,Y1,QA,QB,QC)
      DO 57 I=1,3
      QX(J,IC,I,IB) = QA(I) + D1*(QB(I) - QA(I)) + D2*(QC(I) - QB(I))
   57 CONTINUE
   60 CONTINUE
      RETURN
  200 CONTINUE
      K2 = K1 + IGRD
      K3 = K2 + 1
      IQI = 5
      AAA = D1
      D1 = D2
      D2 = AAA
      GO TO 50
      END
      SUBROUTINE QCOMB(IX,IY,QD)
      DIMENSION DISTX(200,3),XDCAY(600,3),SSIGZ(200,3),EXPOZ(600,3)
     1,HA(5),UHA(5),QXY(5),Q(3600),QX(200,3,3,3),NQX(3,3)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE,XMAX,CON
     1,DECAY,INDEX,THTA,CIGMX,GX,GY, DLTA,IND,SIGY,SIGZ,XR,YR,ZR,XS,YS
     2,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,    NH,HA,UHA
     1, QXY,Q    ,CONC,NH1,QX,NQX
      IF (IX - 8) 20,10,10
   10 CONTINUE
      NX = 2
      GO TO 30
   20 CONTINUE
      NX = 4
   30 CONTINUE
      IF (IY) 31,31,32
   31 CONTINUE
      IY1 = 1
      GO TO 33
   32 CONTINUE
      IY1 = IY
   33 CONTINUE
      IF (IX) 34,34,35
   34 CONTINUE
      IX1 = 1
      GO TO 36
   35 CONTINUE
      IX1 = IX
   36 CONTINUE
      K1 = 120 * (IY1- 1) + 4 *(IX1- 1) - 30
      QD = 0.
      DO 50 J=1,4
      K1 = K1 + 30
      DO 40 I=1,NX
      K = K1 + I
      QD = QD + Q(K)
   40 CONTINUE
   50 CONTINUE
      QD = QD / (4. * NX)
      RETURN
      END
```

```
      SUBROUTINE DISTC
C ROUTINE TO SET DISTANCE DEPENDENT ARRAYS.
      DIMENSION DISTX(200,7),XDCAY(600,7),SSIGZ(200,7),EXPOZ(600,7)
     1,HA(5),UHA(5),QXY(5),Q(3600),QX(200,3,1,7),NQX(7,3)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE,XMAX,CON
     1,DECAY,INDEX,THTA,CIGMX,GX,GY, DLTA,IND,SIGY,SIGZ,XR,YR,ZR,XS,YS
     2,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,    NH,HA,UHA
     1, QXY,Q    ,CONC,NH1,QX,NQX
      COMMON/WNDSP/WSPD,WHGT,PWIND
      NXZLM = 600
C SET ARRAYS WHICH DEPEND ON DISTANCE AND METEOROLOGICAL CONDITIONS ONL
C GET AREA SOURCE WIND SPEEDS FOR EACH EMISSION HEIGHT
      DO 40 IH=1,NH
      UHA(IH) =WSPD* (HA(IH)/WHGT)**PWIND
   40 CONTINUE
```

```
      DO 200 IB=1,7
      NLI = NOX(IB,ICX)
C CHECK THAT DIMENSION LIMIT NXZLM IS NOT EXCEEDED
      NHLI=NH*NLI
      IF (NHLI-NXZLM) 26,26,25
   25 CONTINUE
      WRITE (IPRTR,1004)NXZLM,NHLI
 1004 FORMAT('  NH * NLI     EXCEEDS DIMENSION LIMIT OF',I6,',    NH,=',
     16,',    NLI=',I6)
      IERR = 1
      RETURN
   26 CONTINUE
C GET TRAVEL DISTANCE DECAY FACTORS
      IK = 0
      DO 60 I=1,NLI
      XI = DISTX(I,IB)
      DO 50 IH=1,NH
      IK = IK + 1
      IF (DECAY) 42,42,44
   42 CONTINUE
      XDCAY(IK,IB) = 1.
      GO TO 46
   44 CONTINUE
      XARG = DECAY * XI / UHA(IH)
      IF (XARG - 25.) 45,45,62
   45 CONTINUE
      XDCAY(IK,IB) = EXP(-XARG)
   46 CONTINUE
   50 CONTINUE
   60 CONTINUE
      GO TO 65
   62 CONTINUE
      IL = NH * NLI
      DO 64 I=IK,IL
      XDCAY(I,IB) = 0.
   64 CONTINUE
   65 CONTINUE
      NXI = NLI
C GET SIGMAZ PARAMETERS
      DO 130 I=1,NXI
      XW = DISTX(I,IB)
      CALL SIGZZ
      IF (IERR) 67,68,67
   67 CONTINUE
      RETURN
   68 CONTINUE
      SSIGZ(I,IB) = SIGZ
      IF(SIGZ-CIGMX)70,140,140
   70 CONTINUE
  130 CONTINUE
      KUTEX = NXI
      GO TO 160
  140 CONTINUE
      KUTEX = I
      DO 150 J=I,NXI
      SSIGZ(J,IB) = CIGMX
  150 CONTINUE
  160 CONTINUE
  200 CONTINUE
      RETURN
      END
      SUBROUTINE EXPZC
C ROUTINE TO COMPUTE VERTICAL DIFFUSION FACTOR INCLUDING EFFECTS OF
C    DECAY AND GROUND REFLECTIONS FOR EACH OF NH SOURCE HEIGHTS.
C BASIC EQUATION IS
C          EXPOZ = ( XDCAY / SIGZ )*(EXP(-0.5*((HA-ZR)/SIGZ)**2) +
C                                    EXP(-0.5*((HA+ZR)/SIGZ)**2))
C
      DIMENSION DISTX(200,7),XDCAY(600,7),SSIGZ(200,7),EXPOZ(600,7)
     1,HA(5),UHA(5),QXY(5),Q(3600),QX(200,3,1,7),NQX(7,3)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE,XMAX,CONX
     1,DECAY,INDEX,THTA,CIGMX,GX,GY, DLTA,IND,SIGY,SIGZ,XR,YR,ZR,XS,YS
     2,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,   NH,HA,UHA
     1, QXY,Q    ,CONC,NH1,QX,NQX
C INPUTS
C               ZR = RECEPTOR HEIGHT
C               NH = NUMBER OF SOURCE HEIGHTS
C               HA = ARRAY OF SOURCE HEIGHTS
C            CIGMX = MIXING CEILING
C            SSIGZ = VERTICAL DIFFUSION PARAMETER
C OUTPUT
C            EXPOZ = VERTICAL DIFFUSION FACTOR
C
      DO 100 IB=1,7
      NXI = NQX(IB,ICX)
      K = 0
      DO 60 J=1,NXI
      G = 2. *CIGMX/SSIGZ(J,IB)
      DO 50 I=1,NH
      F = (HA(I) - ZR) /SSIGZ(J,IB)
      IF (F*F -  50.) 12,12,10
   10 CONTINUE
      E1 = 0
   11 CONTINUE
      E2 = 0
      GO TO 15
   12 CONTINUE
      E1 = EXP(-0.5 * F * F)
      F = (HA(I) + ZR) /SSIGZ(J,IB)
      IF (F- 7.) 13,13,11
   13 CONTINUE
      E2 = EXP(-0.5 * F * F)
   15 CONTINUE
      K = K + 1
      EXPOZ(K,IB) = ((E1 + E2)      / SSIGZ(J,IB)) * XDCAY(K,IB)
   50 CONTINUE
   60 CONTINUE
      NX = NXI
  100 CONTINUE
      RETURN
      END


      SUBROUTINE OUTSE
      DIMENSION CNCT(50),CAREA(50),CPOIN(50),XRR(50),YRR(50),ZRR(50)
     1,OBSO2(50),OSET(12,54)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE,XMAX,CONX
     1,DECAY,INDEX,THTA,CIGMX,GX,GY, DLTA,IND,SIGY,SIGZ,XR,YR,ZR,XS,YS
     2,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
     2,XW,YW,ICARD,ICX
      COMMON/OUTPUT/YEAR,AMON,DAY,HOUR ,NRECP,CNCT,CAREA,CPOIN,XRR,YRR
     1,ZRR,OBSO2,IDOW,NR1,TEMP,SIGA,RIB,PCPN,WGLD,STAPR,OSET,INDO
      DATA J1/1/
      WRITE(12) (J,(OSET(I,J-J1+1),I=1,12),J=J1,INDO)
      WRITE(IPRTR,1000) J1,INDO
 1000 FORMAT(' SETS',I6,' TO',I6,' ENTERED IN SENSITIVITY OUTPUT FILE')
      J1 = INDO + 1
      RETURN
      END
      SUBROUTINE CONTRS(J,I1,I2)
      DIMENSION DISTX(200,7),XDCAY(600,7),SSIGZ(200,7),EXPOZ(600,7)
     1,HA(5),UHA(5),QXY(5),Q(3600),QX(200,3,1,7),NQX(7,3)
      DIMENSION SXI(5),        TERMA(5)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE,XMAX,CO
     1,DECAY,INDEX,THTA,CIGMX,GX,GY, DLTA,IND,SIGY,SIGZ,XR,YR,ZR,XS,YS
     2,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/AREAS/NXI,NX,KUTEX,DISTX,XDCAY,SSIGZ,EXPOZ,    NH,HA,UHA
     1, QXY,Q    ,CONC,NH1,QX,NQX
C CONST = 1/(2*SQRT(2*PI))
      DATA CONST/0.199471/
      YW = 0.
      NX = NQX(I2,J)
      DO 10 IH=1,NH
      SXI(IH) = 0
      TERMA(IH) = 0
   10 CONTINUE
      XWL = DISTX(1,I2)
      DO 110 I=1,NX
      XW = DISTX(I,I2)
      IF (NH - 1) 40,40,50
   40 CONTINUE
      QXY(1) = QX(I,J,I1,I2)
      GO TO 60
   50 CONTINUE
      QXY(2) = 0.5 * QX(I,J,I1,I2)
      QXY(1) = 0.5 * QXY(2)
      QXY(3) = QXY(1)
   60 CONTINUE
      DO 90 IH=1,NH
      K = (I -1) * NH + IH
      IF (QXY(IH) - 1.E-50) 70,70,80
   70 CONTINUE
      TERMB = 0.
      GO TO 85
   80 CONTINUE
      TERMB = QXY(IH) * EXPOZ(K,I2)
   85 CONTINUE
      SXI(IH) = SXI(IH) + (TERMA(IH) + TERMB) * (XW - XWL)
      TERMA(IH) = TERMB
   90 CONTINUE
  100 CONTINUE
      XWL = XW
  110 CONTINUE
      IX = NX + 1
      IF (IX - NLI) 115,115,140
  115 CONTINUE
      XW = DISTX(IX,I2)
  120 CONTINUE
      DO 130 IH=1,NH
      SXI(IH) = SXI(IH) + TERMA(IH) * (XW - XWL)
  130 CONTINUE
  140 CONTINUE
      CONC = 0
      DO 150 IH=1,NH
      CONC = CONC + SXI(IH) / UHA(IH)
  150 CONTINUE
      CONC = CONST * CONC
      RETURN
      END
```

Exhibit D-3

LISTING OF FORTRAN CODE SUBROUTINES USED WITH BOTH VALIDATION AND SENSITIVITY PROGRAMS

```
      SUBROUTINE POINT
C       DUE TO EMISSIONS FROM SPECIFIED  POINT SOURCES
C  BASIC EQUATION IS
C           CONP1 =(Q/(2*PI*U*SIGY*SIGZ))*EXP(-0.5*(Y/SIGY)**2-DECAY*X/U)
C                   *(EXP(-0.5*((Z-H)/SIGZ)**2)+EXP(-0.5((Z+H)/SIGZ)**2)))
C               U = WSPD*(ZP/WHGT)**PWIND
C            SIGY = HORIZONTAL DIFFUSION PARAMETER
C            SIGZ = VERTICAL DIFFUSION PARAMETER
C               Y = CROSSWIND DISTANCE BETWEEN SOURCE AND RECEPTOR
C               Z = ZR
C               H = ZP
      DIMENSION XP (100),YP (100),ZP (100),QP(100)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      COMMON/WNDSP/WSPD,WHGT,PWIND
      COMMON/POINTS/NPS   ,XP  ,YP  ,ZP  ,QP,CONPS,NPSS
C  INPUTS
C           XR,YR,ZR = RECEPTOR LOCATION IN SOURCE GRID COORDINATES
C                NPS = NUMBER OF POINT SOURCES
C        XSSXP,YP,ZP = ARRAYS OF POINT SOURCE LOCATIONS IN SOURCE GRIDS
C                 QP = POINT SOURCE EMISSION RATE
C               XONE = CLOSEST DISTANCE TO RECEPTOR
C              ISIGD = DIFFUSION PARAMETER OPTION
C              DECAY = DECAY CONSTANT
C               THTA = WIND DIRECTION
C               WSPD = WIND SPEED AT HEIGHT WHGT
C              PWIND = WIND PROFILE PARAMETER
C              INDEX = DIFFUSION STABILITY PARAMETER
C              CIGMX = MIXING CEILING
C  OUTPUTS
C               IERR = ERROR INDICATOR FROM SIGYZ ROUTINE
C              CONPS = CONCENTRATION AT RECEPTOR FROM NPS POINT SOURCES
      DATA PI/3.14159/
      CONPS = 0
      N1 = NPS - NPSS
      DO  50 I =N1,NPS
      HH = ZP (I)
      XS = XP (I)
      YS = YP (I)
      CALL WCORD
      IF(XW -XONE) 40,10,10
   10 CONTINUE
      CALL SIGYZ
      IF (IERR) 20,30,20
   20 CONTINUE
      RETURN
   30 CONTINUE
      IF (HH - 1.) 28,29,29
   28 CONTINUE
      HH = 1.
   29 CONTINUE
      U = WSPD * (HH / WHGT)**PWIND
      CONP1 =QP(I)/(2*PI*U*SIGY*SIGZ)
      FY = YW/SIGY
      FY2 = FY * FY
      IF (FY2 -50.) 32,40,40
   32 CONTINUE
      CONP2 = EXP(-0.5*FY2)
   33 CONTINUE
      FZ1 = (ZR-HH)/SIGZ
      FZ2 = (ZR+HH)/SIGZ
      IF(FZ1 * FZ1 -50.) 35,34,34
   34 CONTINUE
      CONP3 = 0
      GO TO 36
   35 CONTINUE
      CONP3 = EXP(-0.5*FZ1*FZ1)
   36 CONTINUE
      IF (FZ2 -   7.) 38,37,37
   37 CONTINUE
      CONP4 = 0
      GO TO 39
   38 CONTINUE
      CONP4 = EXP(-0.5*FZ2*FZ2)
   39 CONTINUE
      IF (DECAY) 44,44,45
   44 CONTINUE
      CONP6 = 1.
      GO TO 46
   45 CONTINUE
      AAA = DECAY*XW/U
      IF (AAA - 25.) 48,40,40
   48 CONTINUE
      CONP6 = EXP(-AAA)
   46 CONTINUE
      CONP7 = CONP3 + CONP4
      IF (CONP7 - 1.E-10) 40,40,47
   47 CONTINUE
      CONPI = CONP1*CONP2*CONP7*CONP6
      CONPS = CONPS + CONPI
   40 CONTINUE
   50 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SIGYZ
C ROUTINE TO CALL SUBPROGRAM DESIGNATED BY ISIGD
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,SIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
C          ISIGD = INDICATES OPTION FOR DEFINING DIFFUSION PARAMETERS
C                      1 = MCELROY-POOLER PARAMETERS USING TURNER STAB.
C                      2 = MCELROY-POOLER PARAMETERS USING RICHARDSON NO.
C                      3 = MCELROY-POOLER PARAMETERS USING BROOKHAVEN STAB
C                      4 = PASQUILL PARAMETERS USING TURNER STABILITY CAT.
C          DECAY = DECAY CONSTANT (PER SEC)
      IERR = 0
      GO TO  (  400, 500, 600, 700),ISIGD
  400 CONTINUE
      CALL        SIGY1
      CALL        SIGZ1
      GO TO 800
  500 CONTINUE
      CALL        SIGY2
      CALL        SIGZ2
      GO TO 800
  600 CONTINUE
      CALL        SIGY3
      CALL        SIGZ3
      GO TO 800
  700 CONTINUE
      CALL        SIGY4
      CALL        SIGZ4
  800 CONTINUE
      RETURN
      END
      SUBROUTINE SIGY1
C MCELROY-POOLER PARAMETERS BASED ON TURNER-PASQUILL STABILITY CATEGORY
C THE CALCUALTION USES A POWER LAW - A(INDEX)*X**P(INDEX)
C INPUTS-XW IS DISTANCE FROM SOURCE, INDEX IS STABILITY CLASS NUMBER
C RESTRICTION   XW MUST BE POSITIVE
C IF         RESTRICTION IS VIOLATED THE CALCULATION IS NOT MADE AND
C MESSAGE IS RETURNED
      DIMENSION A(5),P(5)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
C VALUES OF A AND P ARE GIVEN IN THE DATA STATEMENTS FOR EACH ARRAY
      DATA A/ 0.,1.42,1.26,1.13,0.992/
      DATA P/0.,.745,0.73,0.71,0.65/
C TEST FOR RESTRICTION
      IF (XW) 10,10,20
   10 CONTINUE
      WRITE(IPRTR,15) XW
   15 FORMAT(1H ,'SUBROUTINE SIGY1 - BAD INPUT------ X =',F15.2)
      IERR = 1
      RETURN
   20 CONTINUE
      SIGY=A(INDEX)*XW**P(INDEX)
      RETURN
      END
```

```
      SUBROUTINE SIGY2
C MCELROY-POOLER PARAMETERS BASED ON RICHARDSON NO.
C THE CALCUALTION USES A POWER LAW - A(INDEX)*X**P(INDEX)
C INPUTS-XW IS DISTANCE FROM SOURCE, INDEX IS STABILITY CLASS NUMBER
C            IERR = ERROR RETURN
C RESTRICTION   XW MUST BE POSITIVE
C IF         RESTRICTION IS VIOLATED THE CALCULATION IS NOT MADE AND
C MESSAGE IS RETURNED
      DIMENSION A(5), P(5)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      DATA A/1.49,1.4,1.26,1.14,0.945/
      DATA P/.761,0.719,0.712,0.698,0.648/
C TEST FOR FIRST RESTRICTION
      IF(XW       )5,5,10
    5 CONTINUE
      WRITE(IPRTR,15) XW
   15 FORMAT(1H ,'SUBROUTINE SIGY2 - BAD INPUT------ X =',F15.2)
      IERR = 1
      RETURN
      SIGY=A(INDEX)*XW**P(INDEX)
      RETURN
      END
      SUBROUTINE SIGY3
C MCELROY-POOLER PARAMETERS BASED ON MODIFIED BROOKHAVEN STABILITY CAT.
C THE CALCUALTION USES A POWER LAW - A(INDEX)*X**P(INDEX)
C INPUTS-XW IS DISTANCE FROM SOURCE, INDEX IS STABILITY CLASS NUMBER
C RESTRICTION   XW MUST BE POSITIVE
C IF        RESTRICTION IS VIOLATED THE CALCULATION IS NOT MADE AND
C MESSAGE IS RETURNED
      DIMENSION A(4),P(4)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      DATA A/1.48425,1.74942,1.50373,1.39026/
      DATA P /.73727,.68741,.66852,.61474/
C TEST FOR FIRST RESTRICTION
      IF (XW) 10,20,20
      WRITE(IPRTR,15) XW
   15 FORMAT(1H ,'SUBROUTINE SIGY3 - BAD INPUT------ X =',F15.2)
      IERR = 1
      RETURN
   20 CONTINUE
      SIGY=A(INDEX)*XW**P(INDEX)
      RETURN
      END

      SUBROUTINE SIGY4
C PASQUILL-GIFFORD CALCULATION FOR SIGY
C THE CALCUALTION USES A POWER LAW - A(INDEX)*X**P
C INPUTS-XW IS DISTANCE FROM SOURCE, INDEX IS STABILITY CLASS NUMBER
C RESTRICTION   XW MUST BE POSITIVE
      DIMENSION A(6)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      DATA A/.3658,.2751,.2089,.1474,.1046,.0722/
      DATA P/  .9031/
C TEST FOR FIRST RESTRICTION
      IF (XW) 10,10,20
   10 CONTINUE
      WRITE(IPRTR,15) XW
   15 FORMAT(1H ,'SUBROUTINE SIGY4 - BAD INPUT------ X =',F15.2)
      IERR = 1
      RETURN
   20 CONTINUE
      SIGY=A(INDEX)*XW**P
      RETURN
      END


      SUBROUTINE GCHEK
C ROUTINE TO DETERMINE IF POINT X,Y IS OUTSIDE RECT. GRID AREA DEFINED
C BY DIAGONAL FROM 0.5*DELTA,0.5*DELTA TO (GX+0.5)*DELTA,(GY+0.5)*DELTA
C     IND=0 FOR ON GRID, IND=-1 FOR OUTSIDE GRID
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      IF (XS- XSMAX) 10,50,50
   10 IF (YS- YSMAX) 20,50,50
   20 CONTINUE
      IF (XS- XYMIN) 50,50,30
   30 CONTINUE
      IF (YS- XYMIN) 50,50,40
   40 CONTINUE
      IND = 0
      RETURN
   50 CONTINUE
      IND = -1
      RETURN
      END
      SUBROUTINE SIGZZ
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      IERR = 0
      GO TO  (  400, 500, 600, 700),ISIGD
  400 CONTINUE
      CALL       SIGZ1
      GO TO 800
  500 CONTINUE
      CALL       SIGZ2
      GO TO 800
  600 CONTINUE
      CALL       SIGZ3
      GO TO 800
  700 CONTINUE
      CALL       SIGZ4
  800 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SIGZ1
C MCELROY-POOLER PARAMETERS BASED ON TURNER-PASQUILL STABILITY CATEGO
C THE CALCUALTION USES A POWER LAW - A(INDEX)*X**P(INDEX)
C INPUTS-XW IS DISTANCE FROM SOURCE, INDEX IS STABILITY CLASS NUMB
C          IERR = ERROR RETURN
C RESTRICTION  - INDEX MUST BE BETWEEN 2 AND 5
C IF        RESTRICTION IS VIOLATED AN ERROR MESSAGE IS RETURNED
      DIMENSION A(5,2),P(5,2)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      DATA A/ 0.,.0926,0.0891,0.0835,0.0777,0.0,0.072,0.169,1.07,1.
      DATA P/.0,1.18,1.11,1.08,0.955,0.0,1.22,1.01,0.682,0.554/
      IF (ISTAR) 90,5,90
    5 CONTINUE
C TEST FOR RESTRICTION
   20 CONTINUE
      IF (5-INDEX) 30,50,50
   30 CONTINUE
      WRITE(IPRTR,35) INDEX
   35 FORMAT(1H ,'SUBROUTINE SIGZ1 - BAD INPUT------ INDEX =',I4)
      IERR = 1
      RETURN
   50 CONTINUE
      IF(INDEX-2) 30,60,60
   60 CONTINUE
      IF(CIGMX)70,70,80
   70 CONTINUE
      WRITE (IPRTR,1000) CIGMX
 1000 FORMAT (' PARAMETER OUT OF RANGE,CIGMX=',F8.1)
      IERR = 1
      RETURN
   80 CONTINUE
C X1 DEFINES DISTANCE FOR WHICH SIGMAZ = 0.5*MIXING CEILING
      DO 82 J=1,2
      B = A(INDEX,J)
      Q = P(INDEX,J)
      X1 = (CIGMX / (2. * B))**(1. / Q)
      IF (X1 - 600.) 83,83,82
   82 CONTINUE
   83 CONTINUE
C X2 DEFINES DISTANCE FOR WHICH SIGMAZ = MIXING CEILING
      DO 85 J=1,2
      B = A(INDEX,J)
      Q = P(INDEX,J)
      X2 = (CIGMX/B)**(1./Q)
      IF (X2 - 600.) 85,85,84
   84 CONTINUE
   85 CONTINUE
      RETURN
   90 CONTINUE
      IF(XW-X1)100,200,200
C X LESS THAN X1, NO MODIFICATION
  100 CONTINUE
C DETERMINE WHICH RANGE XW IS IN
      IF (XW - 600.) 110,110,120
  110 CONTINUE
C FIRST RANGE
      J = 1
      GO TO 130
  120 CONTINUE
C SECOND RANGE
      J = 2
  130 CONTINUE
      B = A(INDEX,J)
      Q = P(INDEX,J)
      SIGZ = B *XW**Q
      RETURN
  200 CONTINUE
      IF (XW - X2)   300,400,400
C X BETWEEN X1 AND X2
  300 CONTINUE
      SIGZ = 0.5 * CIGMX * (XW + X2 - 2.*X1)/(X2 - X1)
      RETURN
C X GREATER THAN X2
  400 CONTINUE
      SIGZ= CIGMX
      RETURN
      END
      SUBROUTINE SIGZ2
C MCELROY-POOLER PARAMETERS BASED ON RICHARDSON NO.
C THE CALCUALTION USES A POWER LAW - A(INDEX)*X**P(INDEX)
C INPUTS-XW IS DISTANCE FROM SOURCE, INDEX IS STABILITY CLASS NUMBER
C           IERR = ERROR RETURN
C RESTRICTION     INDEX MUST BE BETWEEN 1 AND 5
      DIMENSION A(5,2),P(5,2),C(5)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      DATA A/2*.118,0.115,0.11,0.0954,2*0.00724,0.0581,0.11,0.478/
      DATA P/2*1.02,1.,0.934,0.907,2*1.51,1.12,0.934,0.655/
      DATA C/3*300.,10000.,600./
      IF (ISTAR) 90,5,90
    5 CONTINUE
C TEST FOR RESTRICTION
      IF (5-INDEX) 30,50,50
   30 CONTINUE
      WRITE(IPRTR,35) INDEX
   35 FORMAT(1H ,'SUBROUTINE SIGZ2 - BAD INPUT------ INDEX =',I4)
      IERR = 1
      RETURN
   50 CONTINUE
      IF(INDEX-1) 30,60,60
   60 CONTINUE
      IF(CIGMX)70,70,80
   70 CONTINUE
      WRITE (IPRTR,1000) CIGMX
 1000 FORMAT (' PARAMETER OUT OF RANGE,CIGMX=',F8.1)
      IERR = 1
      RETURN
   80 CONTINUE
C X1 DEFINES DISTANCE FOR WHICH SIGMAZ = 0.5*MIXING CEILING
      DO 82 J=1,2
      B = A(INDEX,J)
      Q = P(INDEX,J)
      X1 = (CIGMX / (2. * B))**(1. / Q)
      IF (X1 - C(INDEX)) 83,83,82
   82 CONTINUE
   83 CONTINUE
C X2 DEFINES DISTANCE FOR WHICH SIGMAZ = MIXING CEILING
      DO 85 J=1,2
      B = A(INDEX,J)
      Q = P(INDEX,J)
      X2 = (CIGMX/B)**(1./Q)
      IF (X2 - 600.) 85,85,84
   84 CONTINUE
   85 CONTINUE
      RETURN
   90 CONTINUE
      IF(XW-X1)100,200,200
C X LESS THAN X1, NO MODIFICATION
  100 CONTINUE
C DETERMINE WHICH RANGE XW IS IN
      IF (XW - C(INDEX)) 110,110,120
  110 CONTINUE
C FIRST RANGE
      J = 1
      GO TO 130
  120 CONTINUE
C SECOND RANGE
      J = 2
  130 CONTINUE
      B = A(INDEX,J)
      Q = P(INDEX,J)
      SIGZ = B *XW**Q
      RETURN
  200 CONTINUE
```

```
      IF (XW - X2)   300,400,400
C X BETWEEN X1 AND X2
  300 CONTINUE
      SIGZ = 0.5 * CIGMX * (XW + X2 - 2.*X1)/(X2 - X1)
      RETURN
C X GREATER THAN X2
  400 CONTINUE
      SIGZ= CIGMX
      RETURN
      END




      SUBROUTINE SIGZ3
C MCELROY-POOLER PARAMETERS BASED ON MODIFIED BROOKHAVEN STABILITY CAT.
C THE CALCUALTION USES A POWER LAW - A(INDEX)*X**P(INDEX)
C INPUTS-XW IS DISTANCE FROM SOURCE, INDEX IS STABILITY CLASS NUMBER
C RESTRICTION    INDEX MUST BE BETWEEN 1 AND 4
C IF EITHER RESTRICTION IS VIOLATED THE CALCULATION IS NOT MADE AND
C MESSAGE IS RETURNED
      DIMENSION A(4),P(4)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      DATA A/.04952,.00837,.11285,.52039/
      DATA P/1.14047,1.48884,.9332,.64672/
      IF (ISTAR) 90,5,90
    5 CONTINUE
C TEST FOR RESTRICTION
      IF (4-INDEX) 30,50,50
   30 CONTINUE
      WRITE(IPRTR,35) INDEX
   35 FORMAT(1H ,'SUBROUTINE SIGZ3 - BAD INPUT------ INDEX =',I4)
      IERR = 1
      RETURN
   50 CONTINUE
      IF (INDEX-1) 30,60,60
   60 CONTINUE
      IF(CIGMX)70,70,80
   70 CONTINUE
      WRITE (IPRTR,1000) CIGMX
 1000 FORMAT (' PARAMETER OUT OF RANGE,CIGMX=',F8.1)
      IERR = 1
      RETURN
   80 CONTINUE
      B=A(INDEX)
      Q=P(INDEX)
C X1 DEFINES DISTANCE FOR WHICH SIGMAZ = 0.5*MIXING CEILING
      RETURN
   90 CONTINUE
      IF(XW-X1)100,200,200
C X LESS THAN X1, NO MODIFICATION
  100 CONTINUE
      SIGZ = B *XW**Q
      RETURN
  200 CONTINUE
      IF (XW - X2)   300,400,400
C X BETWEEN X1 AND X2
  300 CONTINUE
      SIGZ = 0.5 * CIGMX * (XW + X2 - 2.*X1)/(X2 - X1)
      RETURN
C X GREATER THAN X2
  400 CONTINUE
      SIGZ= CIGMX
      RETURN
      END
      SUBROUTINE SIGZ4
C PASQUILL-GIFFORD CALCULATION FOR SIGZ
C THIS CALCULATION USES A POWER LAW - A*X**P
C INPUTS-XW IS DISTANCE FROM SOURCE, INDEX IS STABILITY CLASS NUMBER
C RESTRICTION     INDEX MUST BE BETWEEN 1 AND 5
      DIMENSION A(5,3),P(5,3),C(5,2)
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      DATA A/.125,0.119,0.111,0.105,0.1,0.00883,0.0579,0.111,0.392,0.373
     1,0.000226,0.0579,0.111,.948,2.86/
      DATA P/1.03,0.986,0.911,0.827,0.778,1.51,1.09,0.911,0.636,0.587
     1,2.1,1.09,0.911,0.540,0.366/
      DATA C/250.,4*1000.,500.,4*10000./
      IF( ISTAR  ) 84,5,84
    5 CONTINUE
C TEST FOR RESTRICTION
      IF(5-INDEX) 30,50,50
   30 CONTINUE
      WRITE(IPRTR,35) INDEX
   35 FORMAT (1H ,'SUBROUTINE SIGZ4 - BAD INPUT------ INDEX =',I4)
      IERR = 1
   40 RETURN
   50 CONTINUE
      IF(INDEX-1) 30,60,60
   60 CONTINUE
      IF(CIGMX)70,70,80
   70 CONTINUE
      WRITE (IPRTR,1000) CIGMX
 1000 FORMAT (' PARAMETER OUT OF RANGE,CIGMX=',F8.1)
      IERR = 1
      RETURN
   80 CONTINUE
C X1 DEFINES DISTANCE FOR WHICH SIGMAZ = 0.5*MIXING CEILING
      DO 82 J=1,3
      B=A(INDEX,J)
      Q=P(INDEX,J)
      X1 = (CIGMX/(2.*B))**(1./Q)
      IF ( J - 3) 81,81,83
   81 CONTINUE
      IF (X1 - C(INDEX,J))  83,83,82
   82 CONTINUE
   83 CONTINUE
C X2 DEFINES DISTANCE FOR WHICH SIGMAZ = MIXING CEILING
      DO 92 J=1,3
      B=A(INDEX,J)
      Q=P(INDEX,J)
      X2 = (CIGMX/B)**(1./Q)
      IF (J - 3) 91,91,93
   91 CONTINUE
      IF (X2 - C(INDEX,J)) 93,93,92
   92 CONTINUE
   93 CONTINUE
      RETURN
   84 CONTINUE
      IF (XW - X1) 86,200,200
C XW LESS THAN X1, NO MODIFICATION
C DETERMINE WHICH RANGE X IS IN
   86 CONTINUE
      IF (XW - C(INDEX,J)) 85,85,90
   85 CONTINUE
C J=1 INDICATES THAT X IS IN THE FIRST RANGE
      J=1
      GO TO 120
   90 IF (XW - C(INDEX,J)) 100,110,110
  100 CONTINUE
C J=2 INDICATES THAT X IS IN THE SECOND RANGE
      J=2
      GO TO 120
  110 CONTINUE
C J=3 INDICATES THAT X IS IN THE THIRD RANGE
      J=3
  120 CONTINUE
      SIGZ= A(INDEX,J)*XW**P(INDEX,J)
      RETURN
  200 CONTINUE
      IF (XW - X2)   300,400,400
C X BETWEEN X1 AND X2
  300 CONTINUE
      SIGZ = 0.5 * CIGMX * (XW + X2 - 2.*X1)/(X2 - X1)
      RETURN
C X GREATER THAN X2
  400 CONTINUE
      SIGZ= CIGMX
      RETURN
      END



      SUBROUTINE SCORD
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      IF (ISTAR) 20,10,20
   10 CONTINUE
      ALPH=3.14159/2.- THTA
      COSA = COS(ALPH)
      SINA = SIN(ALPH)
      RETURN
   20 CONTINUE
      XS = XR + XW * COSA - YW * SINA
      YS = YR + XW * SINA + YW * COSA
      RETURN
      END



      SUBROUTINE WCORD
C THIS ROUTINE CONVERTS GRID COORDINATES ON STANDARD GRID REF. SYSTEM TO
C COORDINATES IN A SYSTEM WITH THE X AXIS ALIGNED WITH THE WIND.
C THTA IS WIND DIRECTION ALPHA IS THE ANGLE OF ROTATION FROM STANDARD
C   TO WIND ORIENTED SYSTEM
      COMMON/BASIC/IPRTR,ISTAR,IERR,ISIGD,NXLIM,NXZLM,NLI,XONE
     1,XMAX,CONX,DECAY,INDEX,THTA,CIGMX,GX,GY,DLTA,IND,SIGY
     2,SIGZ,XR,YR,ZR,XS,YS,XW,YW,ICARD,ICX,XYMIN,XSMAX,YSMAX
      IF (ISTAR) 20,10,20
   10 CONTINUE
      ALPHA=3.14159/2.- THTA
      COSA = COS (ALPHA)
      SINA = SIN (ALPHA)
      RETURN
   20 CONTINUE
      XP1 = (XS-XR)*COSA
      XP2 = (YS-YR)*SINA
      XW = XP1 + XP2
      YP1 =(YS-YR)*COSA
      YP2 =(XS-XR)*SINA
      YW  =  YP1 - YP2
      RETURN
      END
```

Appendix E

SAMPLES OF VALIDATION DATA LISTINGS

This appendix describes and presents samples of the punched cards and computer printouts which were generated in the course of this study and which were reviewed to determine results and findings. Since the total set of all pages of computer printouts consists of several thousand pages, only samples of each type of printout are reproduced here.

Two input data records were formed for each hour of validation data. These data records are stored on magnetic tape and may be loaded into disk files for convenient retrieval. An example of the information contained in each record is shown by Figures E-1 and E-2. Figure E-1 lists meteorological parameters, time and date information, sampler observations, and point source emission information which are available in one hourly input record. A description of the computer printout identifications shown in the figure is given in Table E-1. Figure E-2 is a map of hourly area source emission rates obtained from the second type of hourly input record. These figures are samples of the computer printouts generated to review input data for each hour of validation data.

Figures E-3 and E-4 are samples of the map printed for each short-term (two-hour for St. Louis, one-hour for Chicago) validation period. The X's show the relation of sampler locations relative to one another. The upper printed number by each X is the observed value, and the lower printed number is the predicted value. Stars designate missing values. The principal meteorological inputs are also shown.

```
   REC.ID   DOW    TEMP   SIGA    RIR     PCPN  WGUST    PRESS    NR1
     214.     4    34.0  999.0********     2.00     0.   27.74      40

 YEAR AMON  DAY HOUR NRECP GX    GY   DELTA  NH NRPNT  USPD  UHGT PWIND  THTA INDEX  CIGMX
  64.  12.   2.  14.    50 30.  40.   1524.   3   51   3.70  20.8 0.128 1.500   4    441.

OBS        381.000    222.000    126.000    152.000    999.000    114.000    362.000    116.000    104.000
OBS        129.000     39.000    100.000    110.000    174.000    174.000    290.000    101.000    999.000
OBS         84.000     51.000     22.000      6.000    173.000     19.000    259.000     40.000    104.000
OBS        159.000     23.000     97.000     29.000     34.000    999.000     85.000    125.000     72.000
OBS        293.000   9999.000    410.000     19.000    236.000   9999.000   9999.000     90.000   9999.000

               1          2          3          4          5          6          7          8
QP      0.806E+02  0.278E+03  0.318E+02  0.429E+03  0.173E+02  0.179E+03  0.323E+02  0.476E+03
ZP          40.00     239.93      40.00     111.34      40.00     101.15      40.00     146.39

              11         12         13         14         15         16         17         18
QP      0.152E+03  0.334E+02  0.172E+02  0.764E+02  0.645E+01  0.172E+02  0.173E+02  0.142E+02
ZP         152.28      40.00      40.00      40.00      40.00      49.00      19.00      47.00

              21         22         23         24         25         26         27         28
QP      0.293E+02  0.305E+03  0.610E+02  0.123E+03  0.166E+02  0.132E+03  0.163E+03  0.144E+02
ZP          75.00     125.00      55.00      73.38      75.00      97.25      99.31      55.00

              31         32         33         34         35         36         37         38
QP      0.337E+03  0.110E+03  0.761E+02  0.217E+02  0.184E+03  0.559E+03  0.586E+03  0.256E+02
ZP         167.20      55.00      55.00      75.00      79.10     210.12     300.80      75.00

              41         42         43         44         45         46         47         48
QP      0.353E+03  0.529E+03  0.706E+03  0.268E+04  0.682E+03  0.682E+03  0.128E+04  0.167E+04
ZP         106.87     122.21     134.79     328.06     257.16     257.16     399.66     463.70

              51
QP      0.564E+03
ZP         197.64
```

Figure E-1. Sample Hourly Input Data Set of Meteorological and Point Source Parameters

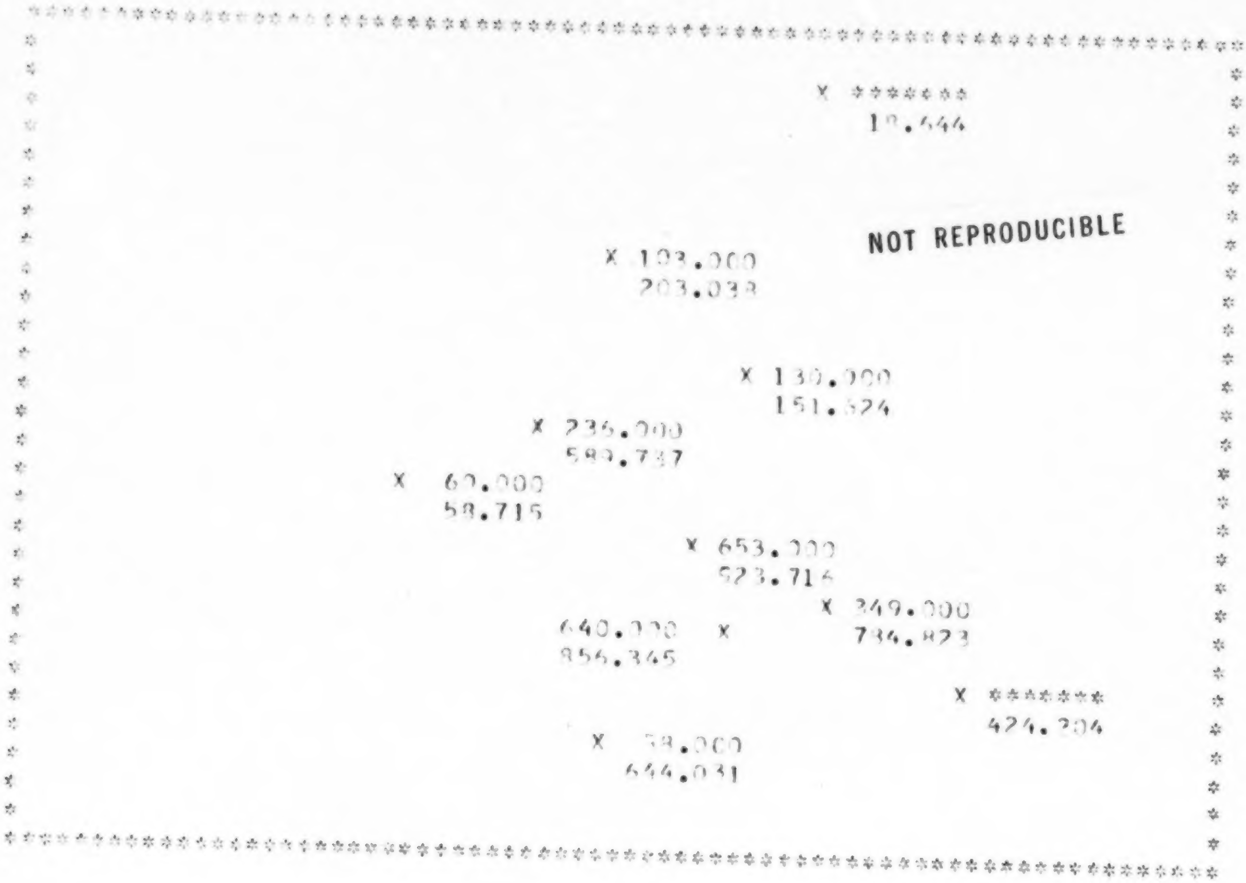
```
               ST. LOUIS AREA SOURCE EMISSION RATES

   0 -    0.0    TO    0.01         6 -     3.00+ TO   10.00
   1 -    0.01+  TO    0.03         7 -    10.00+ TO   30.00
   2 -    0.03+  TO    0.10         8 -    30.00+ TO  100.00
   3 -    0.10+  TO    0.30         9 - OVER 100.00
   4 -    0.30+  TO    1.00
   5 -    1.00+  TO    3.00

                          115.

                1         2         3
       123456789012345678901234567890
     1 344444444233303333344444444444
     2 334444444323333343344444444444
     3 334444444342333333455434440444
     4 344444444444244455554444444444
     5 333444444344300055554444444444
     6 333444454444425555554444444444
     7 333344334444430055444445644444
     8 333333444444430555444444434444
     9 333333444444433344444444444044
    10 333333444445532045444344444455
    11 333344444455652006444444444357
    12 444444454555575445444444444476
    13 454434655556677254544444444677
    14 466434665666767704555554445667
    15 444455656656767860555465448555
    16 444456656666667787545266656555
    17 444466657676777888447865777555
    18 334444356777778888878887555555
    19 434444336777777888768987755555
    20 444455555677658898856857755555
    21 333345444677888988764556655477
    22 433345454567888888776520555467
    23 834334555666688888677644444435
    24 333344566566677865267644044344
    25 333345667776677760067864444044
    26 333355666666667770026664444044
    27 233355665777556566004544444434
    28 203355565576665547304444544444
    29 320123365456655543443455554444
    30 570234444556554444450455550444
    31 676445554335444455430044444444
    32 255044444434444444440024444444
    33 332204233433344444400021044444
    34 033220203333333333000006603224
    35 333322333233333332220022611333
    36 223332232223333223333022360033
    37 333333333300023333222326754333
    38 333333333300033332577767553333
    39 033332323333333323787862462444
    40 022333223332330224766680665533
```

Figure E-2. Sample Map of Hourly Area Source Emission Rates

Table E-1. Description of Computer Printout Identifications

Identification	Description
REC. ID	Record identification number
DOW	Day of the week
TEMP	Ambient air temperature (°F)
SIGA	Standard deviation in horizontal wind direction
RIB	Bulk Richardson number
PCPN	Precipitation in 0.01 in/hr
WCUST	Peak wind gust, knots
PRESS	Atmospheric pressure, in Hg
NRI	= 40, number of 24-hour samplers
AMON	Month of the year
DAY	Day of the month
NRECP	= 50, number of 24-hour and 2-hour samplers
GX	Number of East-West coordinates in area source grid
GY	Number of North-South coordinates in area source grid
DELTA	Spacing between area source grid points, m
NH	= 3, number of area source heights
NRPNT	Number of point sources
USPD	Wind speed at height UHGT, m/sec
UHGT	Reference height for wind speed, m
PWIND	Wind profile exponent
THTA	Wind direction, radians from North
INDEX	Stability class for diffusion parameters
CIGMX	Mixing ceiling, m
OBS	Observed SO_2 concentration, $\mu g/m^3$ (first 40 are 24-hour average, last 10 are 2-hour average)
QP	Point source emission rate, g/sec
ZP	Effective point source height, m

ST LOUIS DATA

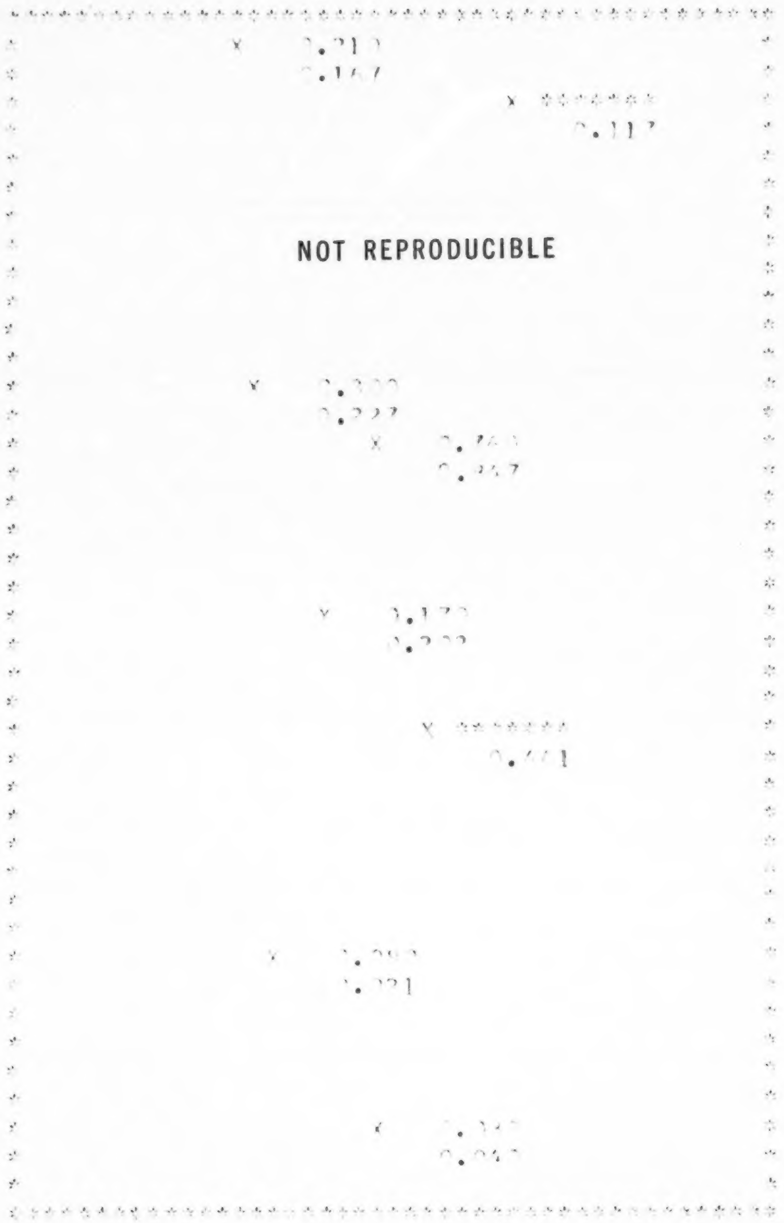

X ******
19.644
X 103.000
203.038
X 130.000
151.524
X 236.000
589.737
X 60.000
58.715
X 653.000
523.716
X 349.000
734.823
640.000 X
856.345
X ******
424.204
X 38.000
644.031

NOT REPRODUCIBLE

```
                                     HOUR 5.        HOUR 6.

WIND DIRECTION  (DEGREES)             -34.4          -45.8
WIND SPEED      (M/SEC )                2.9            1.9
STABILITY CLASS                         5              5
TEMPERATURE     (DEG,C  )              13.0           13.0
MIX.CEILING     (METERS)              352.0          352.0
PRECIPITATION                           0.0            0.0
```

Figure E-3. Sample Computer Generated Map Used to Review St. Louis Validation Results

CHICAGO DATA


0.210
0.167
0.117
0.227
0.247
0.441
0.221

NOT REPRODUCIBLE

```
WIND DIRECTION (DEGREES)        174.[illegible]
WIND SPEED     (M/SEC)            [illegible]
STABILITY CLASS                    [illegible]
TEMPERATURE    (DEG,C)           12.[illegible]
MIX.CEILING    (METERS)         [illegible]
PRECIPITATION                      [illegible]
```

Figure E-4. Sample Computer Generated Map Used to Review Chicago Validation Results

Figure E-5 is an example of the statistical summary of validation results for a single Chicago station (90 and 100 percent values of the frequency distribution are not shown in this example although they are included in complete computer printout). Similar summaries were generated for each observing location and for all stations combined. Summaries were generated for the entire validation period and for selected subsets of the period, e.g., all hours for which the wind speed had some specified range.

The validation results are also available on punched cards. The format for the punched card data is listed in Table E-2.

```
                         STATISTICAL SUMMARY FOR    1  STATIONS
                         BEGINNING DATE   67.   1.   1.   0.
                         ENDING    DATE   67.   1.  31.  23.


                         STATION INDEX NUMBERS USED IN THIS RUN ARE
                                        1
                NUMBER                     SUM OF
               OF CASES        SUM         SQUARES                      STANDARD      MEAN ABSOLUTE
                                                            MEAN        DEVIATION       DIFFERENCE

       OBSERVED     673   0.22119E 02   0.29168E 01    0.32866E-01   0.57085E-01
      PREDICTED     673   0.48279E 02   0.14854E 03    0.71737E-01   0.46465E 00
OBSRVD-PREDICTED    673  -0.26162E 02   0.14405E 03   -0.38874E-01   0.46135E 00   0.62249E-01

                        REGRESSION COEFFICIENTS
            SLOPE                  B(1)=      0.0146
            INTERCEPT              B(0)=      0.0318



   DECILE        0        10        20    FREQUENCY DISTRIBUTION BY DECILES
                                             30        40        50        60        70        80
  OBSERVED      0.0       0.0       0.0      0.0      0.010     0.010     0.010     0.030     0.050
 PREDICTED     0.000     0.005     0.007    0.009     0.012     0.014     0.017     0.027     0.042
 OBSERVED
    MINUS
 PREDICTED   -10.913    -0.049    -0.027   -0.015    -0.011    -0.007    -0.004     0.000     0.011
```

Figure E-5. Sample of Statistical Summary of Validation Results

Table E-2. Punch Card Format for Validation Data

I. Format for St. Louis Validation Data at 10 Stations				
Card	Columns	Format*	Units	Description
1	1-8	I8	None	Output record index number
	9-10	I2	None	Day of the week
	11-12	I2	None	= 10
	13-52	10I4	$\mu g/m^3$	Observed concentrations for stations 3, 15, 17, 23, 33, 4, 10, 12, 28 and 36, respectively
	53-76	6I4	$\mu g/m^3$	Calculated concentrations for stations 3, 15, 17, 23, 33 and 4, respectively
	77-79	3X	None	Blank
	80	I1	None	= 1
2	1-8	I8	None	Output record index number
	9-24	4I4	$\mu g/m^3$	Calculated concentrations for stations 10, 12, 28 and 36, respectively
	25-28	F4.1	m/sec	Wind speed for reference height
	29-32	F4.1	m	Wind speed for reference height
	33-36	F4.3	None	Wind profile exponent
	37-40	F4.2	Radians	Wind direction
	41	I1	None	Stability class index
	42-45	F4.1	°F	Air temperature
	46-50	I5	m	Mixing layer ceiling
	51-55	F5.1	°Azimuth	Wind turbulence statistics (σ_A)
	56-62	F7.3	None	Bulk Richardson number
	63-66	F4.2	0.01 in/hr	Precipitation rate
	67-70	F4.1	knots	Peak wind gust
	72-75	F5.2	in Hg	Atmospheric pressure
	77-79	4X	None	Blank
	80	I1	None	= 2

(Continued)

Table E-2. Punch Card Format for Validation Data (Concluded)

II. Format for Chicago Validation Data at 8 Stations				
Card	Columns	Format*	Units	Description
1	1-10			See Part I above
	11	1X	None	Blank
	12	I1	None	= 8
	13-44	8I4	mg/m^3	Observed concentrations for stations 1 to 8, respectively
	45-76	8I4	mg/m^3	Calculated concentrations for stations 1 to 8, respectively
	77-80			See Part I above
2	1-8			See Part I above
	9-24	16X	None	Blank
	25-80			See Part I above

*Standard FORTRAN code notation.

Appendix F

SAMPLES OF SENSITIVITY DATA LISTINGS

This appendix describes and presents samples of the computer printouts which were generated to permit review of the sensitivity results. The total set of all printed results consists of several hundred pages. Only samples of each type of printout are reproduced here.

An output record was generated for each set of input values considered in the sensitivity analysis. A listing of the concentrations and input values for each of 5832 records was made in the format shown in Figure F-1. A description of the computer printout identification in Figure F-1 is given in Table F-1. The sensitivity output records were stored in disk files for subsequent statistical analysis and tabulation of results.

One type of summary which was generated is illustrated in Figure F-2. The mean concentration of all records with a given input value was determined. The results in Figure F-2 are for the entire set of sensitivity results. Similar summaries were generated from selected subsets of the total set of results in order to evaluate special sensitivity considerations.

Another type of listing which provides a convenient review of model sensitivity results is illustrated in Figure F-3. This figure is a partial listing of all comparisons of calculated concentrations in which the only input changed is the mixing ceiling. Similar listings were generated for all inputs considered in the sensitivity analysis.

A quick review of this type of printout easily identifies the combinations of input values (if any) for which "sensitive" results are generated with input parameter.

A specialized type of summary was generated to examine the effects of changes in wind direction input. An example of this specialized printout is given in Figure F-4.

```
INDO TOT. CONC.   ISIGD    INDEX    CIGMX    PWIND     WSPD   DECAY    NH     DLTA    NPS   RECEPTOR

   1  0.291E+02      4        5     100.     0.150      2.0    0.0      1     381.     51    22366.
   2  0.304E+04      4        5     100.     0.150      2.0    0.0      1     381.     51    25146.
   3  0.109E+03      4        5     100.     0.150      2.0    0.0      1     381.     51    30707.
   4  0.291E+02      4        5     100.     0.150      2.0    0.0      1     381.     19    22366.
   5  0.122E+05      4        5     100.     0.150      2.0    0.0      1     381.     19    25146.
   6  0.106E+03      4        5     100.     0.150      2.0    0.0      1     381.     19    30707.
   7  0.291E+02      4        5     100.     0.150      2.0    0.0      1     381.      0    22366.
   8  0.462E+05      4        5     100.     0.150      2.0    0.0      1     381.      0    25146.
   9  0.106E+03      4        5     100.     0.150      2.0    0.0      1     381.      0    30707.
  10  0.360E+02      4        5     100.     0.150      2.0    0.0      1    1524.     51    22366.
  11  0.321E+04      4        5     100.     0.150      2.0    0.0      1    1524.     51    25146.
  12  0.127E+03      4        5     100.     0.150      2.0    0.0      1    1524.     51    30707.
  13  0.360E+02      4        5     100.     0.150      2.0    0.0      1    1524.     19    22366.
  14  0.485E+04      4        5     100.     0.150      2.0    0.0      1    1524.     19    25146.
  15  0.124E+03      4        5     100.     0.150      2.0    0.0      1    1524.     19    30707.
  16  0.360E+02      4        5     100.     0.150      2.0    0.0      1    1524.      0    22366.
  17  0.868E+04      4        5     100.     0.150      2.0    0.0      1    1524.      0    25146.
  18  0.124E+03      4        5     100.     0.150      2.0    0.0      1    1524.      0    30707.
  19  0.420E+02      4        5     100.     0.150      2.0    0.0      1    6096.     51    22366.
  20  0.302E+04      4        5     100.     0.150      2.0    0.0      1    6096.     51    25146.
  21  0.191E+03      4        5     100.     0.150      2.0    0.0      1    6096.     51    30707.
  22  0.433E+02      4        5     100.     0.150      2.0    0.0      1    6096.     19    22366.
  23  0.358E+04      4        5     100.     0.150      2.0    0.0      1    6096.     19    25146.
  24  0.190E+03      4        5     100.     0.150      2.0    0.0      1    6096.     19    30707.
  25  0.433E+02      4        5     100.     0.150      2.0    0.0      1    6096.      0    22366.
  26  0.244E+04      4        5     100.     0.150      2.0    0.0      1    6096.      0    25146.
  27  0.190E+03      4        5     100.     0.150      2.0    0.0      1    6096.      0    30707.
```

Figure F-1. Sample Listing of Computer Records of Sensitivity Results

Table F-1. Description of Computer Printout Identifications

Identification	Description
INDO	Output record index number
TOT. CONC.	Calculated concentration at receptor location, $\mu g/m^3$
ISIGD	Index to designate system of diffusion parameters used
INDEX	Stability index for diffusion parameters
CIGMX	Mixing ceiling, m
PWIND	Wind profile exponent
WSPD	Wind speed at reference height, m/sec
DECAY	Decay constant (inverse of mean decay time), sec
NH	Number of area source heights
DLTA	Spacing between area source grid points, m
NPS	Number of point sources
RECEPTOR	East-West coordinate of receptor location, m

```
PARAMETER                                  VALUE    MEAN CONCENTRATION

RECEPTOR LOCATION (M.,EAST)           0.2237E+05           0.6002E+01
RECEPTOR LOCATION (M.,EAST)           0.2515E+05           0.3856E+03
RECEPTOR LOCATION (M.,EAST)           0.3071E+05           0.3962E+03
NO. OF POINT SOURCES                  0.5100E+02           0.2371E+03
NO. OF POINT SOURCES                  0.1900E+02           0.2616E+03
NO. OF POINT SOURCES                  0.0                  0.2891E+03
AREA SOURCE GRID SPACING (M.)         0.3810E+03           0.2769E+03
AREA SOURCE GRID SPACING (M.)         0.1524E+04           0.2735E+03
AREA SOURCE GRID SPACING (M.)         0.6096E+04           0.2373E+03
NO. AREA SOURCE EMISSION HGTS         0.1000E+01           0.2626E+03
DECAY CONSTANT                        0.0                  0.3921E+03
DECAY CONSTANT                        0.3851E-03           0.1331E+03
WIND SPEED (M/SEC)                    0.2000E+01           0.5112E+03
WIND SPEED (M/SEC)                    0.6000E+01           0.1983E+03
WIND SPEED (M/SEC)                    0.1800E+02           0.7831E+02
WIND PROFILE PARAMETER                0.1500E+00           0.2626E+03
MIXING CEILING (M.)                   0.1000E+03           0.3455E+03
MIXING CEILING (M.)                   0.5000E+03           0.1797E+03
DIFFUSION FUNCTIONS (TYPE)            0.4000E+01           0.3520E+03
DIFFUSION FUNCTIONS (TYPE)            0.1000E+01           0.2188E+03
DIFFUSION FUNCTIONS (TYPE)            0.2000E+01           0.2169E+03
```

Figure F-2. Summary of Sensitivity Results by Input Parameter

```
         CONCENTRATIONS FOR             NO. OF   AREA  NO. OF  DECAY     WIND    WIND
DIFFUS.     MIXING CEILING, M. RECEPTOR POINT    GRID  AREA    CONST     SPEED   POWER
  FN.       100      500       LOCATION SOURCES  MI    HGTS.    /SEC     M/S     LAW

   4         11.      12.       UPWIND    51     0.25    1  0.000          2     0.15
   4       1259.    1635.       CENTER    51     0.25    1  0.000          2     0.15
   4       2061.    1526.     DOWNWIND    51     0.25    1  0.000          2     0.15
   4         11.      12.       UPWIND    19     0.25    1  0.000          2     0.15
   4       1259.    1635.       CENTER    19     0.25    1  0.000          2     0.15
   4       1849.    1376.     DOWNWIND    19     0.25    1  0.000          2     0.15
   4         11.      12.       UPWIND     0     0.25    1  0.000          2     0.15
   4       1259.    1635.       CENTER     0     0.25    1  0.000          2     0.15
   4       1750.    1321.     DOWNWIND     0     0.25    1  0.000          2     0.15
   4         15.      15.       UPWIND    51     1.00    1  0.000          2     0.15
   4       1211.    1212.       CENTER    51     1.00    1  0.000          2     0.15
   4       1987.    1469.     DOWNWIND    51     1.00    1  0.000          2     0.15
   4         15.      15.       UPWIND    19     1.00    1  0.000          2     0.15
   4       1238.    1239.       CENTER    19     1.00    1  0.000          2     0.15
   4       2811.    2124.     DOWNWIND    19     1.00    1  0.000          2     0.15
   4         15.      15.       UPWIND     0     1.00    1  0.000          2     0.15
   4       1238.    1239.       CENTER     0     1.00    1  0.000          2     0.15
   4       2711.    2059.     DOWNWIND     0     1.00    1  0.000          2     0.15
   4         25.      25.       UPWIND    51     4.00    1  0.000          2     0.15
   4        829.     830.       CENTER    51     4.00    1  0.000          2     0.15
   4       1402.    1024.     DOWNWIND    51     4.00    1  0.000          2     0.15
   4         48.      48.       UPWIND    19     4.00    1  0.000          2     0.15
   4       1205.    1207.       CENTER    19     4.00    1  0.000          2     0.15
   4       1738.    1269.     DOWNWIND    19     4.00    1  0.000          2     0.15
   4         48.      48.       UPWIND     0     4.00    1  0.000          2     0.15
   4       1929.    1960.       CENTER     0     4.00    1  0.000          2     0.15
   4       2621.    1899.     DOWNWIND     0     4.00    1  0.000          2     0.15
   4          7.       7.       UPWIND    51     0.25    1  0.000385       2     0.15
   4       1146.    1143.       CENTER    51     0.25    1  0.000385       2     0.15
   4         41.      36.     DOWNWIND    51     0.25    1  0.000385       2     0.15
   4          7.       7.       UPWIND    19     0.25    1  0.000385       2     0.15
   4       1146.    1143.       CENTER    19     0.25    1  0.000385       2     0.15
   4         39.      34.     DOWNWIND    19     0.25    1  0.000385       2     0.15
   4          7.       7.       UPWIND     0     0.25    1  0.000385       2     0.15
   4       1146.    1143.       CENTER     0     0.25    1  0.000385       2     0.15
   4         35.      32.     DOWNWIND     0     0.25    1  0.000385       2     0.15
   4          9.       9.       UPWIND    51     1.00    1  0.000385       2     0.15
   4        785.     784.       CENTER    51     1.00    1  0.000385       2     0.15
   4         36.      31.     DOWNWIND    51     1.00    1  0.000385       2     0.15
```

Figure F-3. Sample Listing of Comparisons for a Selected Variation in a Model Input

```
AREA SOURCE, WIND AZIMUTH IS 349


                                               UNITS ARE MICROGRAMS/CU.M.
                     MIXING   WIND    MODEL
LOCA-     STA-       CEIL.    SPEED   CONCEN-   ABS. ERROR BY WIND ERROR
TION      BILITY     (M)      (M/S)   TRATION    3 DEG     10 DEG    45 DEG

UPWIND    STABLE     100.      2.        12.        1.         2.       66.
CENTER    STABLE     100.      2.      1576.       32.       106.      526.
DNWIND    STABLE     100.      2.      1890.      489.      1247.     1823.
UPWIND    STABLE     100.      6.         4.        0.         1.       22.
CENTER    STABLE     100.      6.       525.       11.        35.      144.
DNWIND    STABLE     100.      6.       630.      163.       416.      607.
UPWIND    STABLE     100.     18.         1.        0.         0.        7.
CENTER    STABLE     100.     18.       175.        4.        12.       48.
DNWIND    STABLE     100.     18.       210.       54.       139.      202.
UPWIND    STABLE     500.      2.        12.        1.         2.       59.
CENTER    STABLE     500.      2.      1566.       29.       107.      453.
DNWIND    STABLE     500.      2.      1422.      360.       935.     1363.
UPWIND    STABLE     500.      6.         4.        0.         1.       20.
CENTER    STABLE     500.      6.       522.       10.        36.      151.
DNWIND    STABLE     500.      6.       474.      120.       312.      454.
UPWIND    STABLE     500.     18.         1.        0.         0.        7.
CENTER    STABLE     500.     18.       174.        3.        12.       50.
DNWIND    STABLE     500.     18.       158.       40.       104.      151.
UPWIND    NEUTRAL    100.      2.         9.        1.         1.       65.
CENTER    NEUTRAL    100.      2.      1063.       33.        60.      245.
DNWIND    NEUTRAL    100.      2.      1879.      487.      1243.     1815.
UPWIND    NEUTRAL    100.      6.         3.        0.         0.       22.
CENTER    NEUTRAL    100.      6.       354.       11.        20.       82.
DNWIND    NEUTRAL    100.      6.       626.      162.       414.      605.
UPWIND    NEUTRAL    100.     18.         1.        0.         0.        7.
CENTER    NEUTRAL    100.     18.       118.        4.         7.       27.
DNWIND    NEUTRAL    100.     18.       209.       54.       138.      202.
UPWIND    NEUTRAL    500.      2.         3.        0.         1.       14.
CENTER    NEUTRAL    500.      2.       571.       68.        30.      173.
DNWIND    NEUTRAL    500.      2.       382.       99.       252.      367.
UPWIND    NEUTRAL    500.      6.         1.        0.         0.        5.
CENTER    NEUTRAL    500.      6.       190.       23.        10.       58.
DNWIND    NEUTRAL    500.      6.       127.       33.        84.      122.
UPWIND    NEUTRAL    500.     18.         0.        0.         0.        2.
CENTER    NEUTRAL    500.     18.        63.        8.         3.       19.
DNWIND    NEUTRAL    500.     18.        42.       11.        28.       41.
UPWIND    UNSTAB     100.      2.         9.        1.         1.       65.
CENTER    UNSTAB     100.      2.      1065.       31.        58.      246.
DNWIND    UNSTAB     100.      2.      1879.      487.      1243.     1815.
UPWIND    UNSTAB     100.      6.         3.        0.         0.       22.
CENTER    UNSTAB     100.      6.       355.       10.        19.       82.
DNWIND    UNSTAB     100.      6.       626.      162.       414.      605.
UPWIND    UNSTAB     100.     18.         1.        0.         0.        7.
CENTER    UNSTAB     100.     18.       118.        3.         6.       27.
DNWIND    UNSTAB     100.     18.       209.       54.       138.      202.
UPWIND    UNSTAB     500.      2.         2.        0.         0.       13.
CENTER    UNSTAB     500.      2.       382.       82.        26.       83.
DNWIND    UNSTAB     500.      2.       379.       98.       250.      365.
UPWIND    UNSTAB     500.      6.         1.        0.         0.        4.
CENTER    UNSTAB     500.      6.       127.       27.         9.       28.
DNWIND    UNSTAB     500.      6.       126.       33.        83.      122.
UPWIND    UNSTAB     500.     18.         0.        0.         0.        1.
CENTER    UNSTAB     500.     18.        42.        9.         3.        9.
DNWIND    UNSTAB     500.     18.        42.       11.        28.       41.

                              MEAN      377.       61.       149.      255.
```

Figure F-4. Sample of Sensitivity Results for Changes in Wind Direction Input